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# Soil Generic Assessment Criteria for Human Health Risk Assessment

January 2010

CONTAMINATED LAND: APPLICATIONS IN REAL ENVIRONMENTS

# CL: AIRE

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# The EIC/AGS/CL:AIRE Soil Generic Assessment Criteria for Human Health Risk Assessment

Environmental Industries Commission  
(EIC)

The Association of Geotechnical and Geoenvironmental  
Specialists (AGS)

Contaminated Land: Applications in Real Environments  
(CL:AIRE)

## Publication

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The contributors to this report are employed by the various companies listed in the Acknowledgments below. The work reported herein was carried out by voluntary agreement between all of these companies and umbrella organisations. Any views expressed are not necessarily those of CL:AIRE, the EIC, the AGS or any of the contributing companies and named individuals. The publication is intended to provide accurate and authoritative information on the generic assessment criteria (GAC) for particular potentially contaminative substances in soil relevant to the assessment of risk to human health by land affected by contamination. However, as set out in the text, it is imperative that users do not refer solely to the GAC values, but they read and understand their derivation and limitations as described in the supporting text presented herein.

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-

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# Introduction



# 1 Introduction

This report presents the results of a collaborative effort of risk assessors from 26 EIC and AGS member companies to produce generic assessment criteria (GAC) for soils for human health risk assessment. The project involved the collation and review of physico-chemical data, toxicological data and information on background exposure for 44 contaminants sometimes encountered on land affected by contamination in the UK and the derivation of GAC for 35<sup>1</sup> of these using the CLEA model (v1.06). The GAC are intended to complement soil guideline values (SGV) produced by the Environment Agency of England and Wales and the 2nd edition GAC produced by LQM and CIEH (Nathanail et al, 2009). All three sets of assessment criteria have been derived in general accordance with the Environment Agency of England and Wales Contaminated Land Exposure Assessment (CLEA) guidance and thus the combined efforts of these three groups have resulted in a useful set of screening criteria for the assessment of risks to human health from soil contamination for more than 120 potentially contaminative substances.

## 1.1 Background

As discussed in the CLR11 Model Procedures report (Environment Agency, 2004) GAC are a useful screening tool in the assessment of risks from land contamination. When used in conjunction with the conceptual site model they can streamline the risk assessment process by reducing the number of contaminants and/or pollutant linkages requiring more detailed risk assessment and in many cases can help to demonstrate that there are no unacceptable risks at a site.

The EIC initiative to derive GAC was initiated in December 2008 after the introduction of the revised CLEA methodology in August of that year. At that time, the Environment Agency of England and Wales had plans to produce SGV for around 15 substances/groups of substances in the forthcoming months. These SGV would provide authoritative screening criteria for the assessment of risks to human health but still represented a relatively small number of the commonly encountered contaminants in UK soils. Two projects were initiated to help fill this gap: the EIC project, presented herein and the LQM/CIEH project. LQM and CIEH, aided by a wide collaboration from the contaminated land community, worked on the derivation of GAC for 82 contaminants through the first half of 2009 and published these in July 2009. The EIC project, also collaborative in nature and supported by AGS and CL:AIRE, was initiated to produce industry agreed GAC to complement those of LQM/CIEH and published SGV.

<sup>1</sup> Note that there were insufficient toxicological data available to derive health criteria values (HCV) that were acceptable to the entire group of risk assessors for nine substances and consequently GAC were not derived for these substances

## 1.2 Aims of the Project

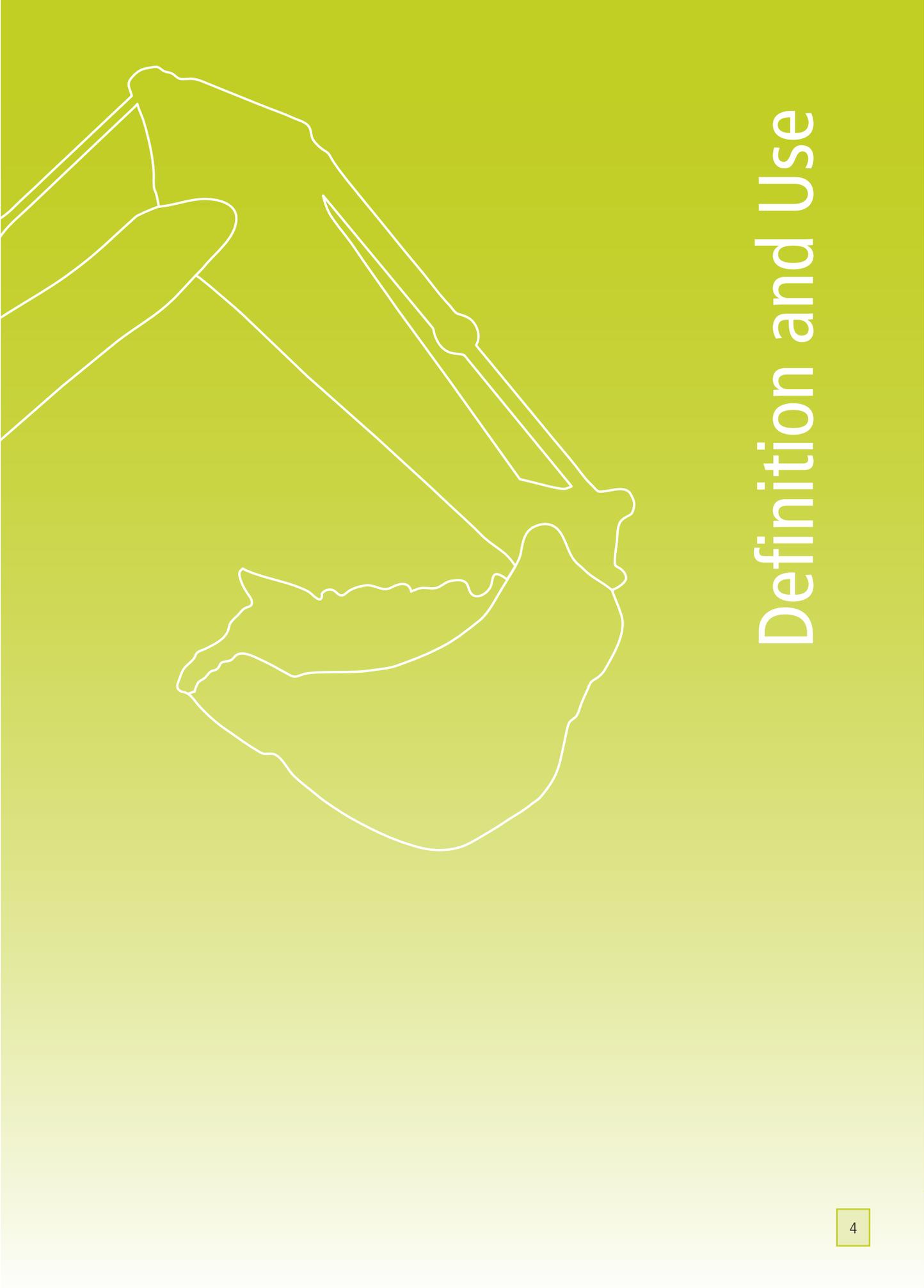
The aims of the EIC/AGS/CL:AIRE GAC project were to:

- derive a set of industry agreed contaminant specific parameter values for input to the CLEA model for a range of commonly encountered contaminants that were not being considered by the Environment Agency of England and Wales or LQM/CIEH;
- derive a set of industry agreed GAC for those contaminants with sufficient appropriate data to do so;
- present the data and assumptions used to derive the GAC in a fully transparent manner to enable practitioners to make their own judgements about the suitability of the recommended values for their specific purposes; and
- provide a spreadsheet of contaminant specific parameter values in electronic format suitable for input to the CLEA model to facilitate the derivation of site specific assessment criteria for the researched contaminants.

## 1.3 Report Structure

The report is structured as follows:

- Chapter 1 – Motivation and aims of the project;
- Chapter 2 – Description of what the EIC/AGS/CL:AIRE are and how these should be used;
- Chapter 3 – Methodology used for derivation of EIC/AGS/CL:AIRE;
- Chapter 4 – The EIC/AGS/CL:AIRE tables;
- Chapter 5 – References;
- Appendix A – Contaminant data inputs for CLEA model; and
- Appendix B – Contaminant proformas.



# Definition and Use

## 2 Definition and Use of EIC/AGS/CL:AIRE GAC

### 2.1 EIC/AGS/CL:AIRE Derived

The EIC/AGS/CL:AIRE have been derived for 3 metals and 32 organic contaminants as listed in Table 2.1.

Table 2.1: Contaminants with EIC/AGS/CL:AIRE GAC

Substance	CAS	Synonyms
<b>Metals</b>		
Antimony	n/a	
Barium	n/a	
Molybdenum	n/a	
<b>Hydrocarbons</b>		
1,2,4-Trimethylbenzene	95-63-6	Pseudocumene; psicumene
Isopropylbenzene	98-82-8	Cumene; 2-phenylpropane
Propylbenzene	103-65-1	<i>n</i> -Propylbenzene; Isocumene; 1-phenylpropane; 1-propylbenzene
Styrene	100-42-5	Vinyl benzene; cinnamene; styrol; phenethylene; phenylethene
<b>Phenols</b>		
2,4-Dimethylphenol	105-67-9	2,4-DMP; 2,4-xylenol; <i>m</i> -xylenol; 1-hydroxy-2,4-dimethylbenzene
2-Methylphenol	95-48-7	<i>o</i> -Cresol; <i>ortho</i> -cresol
3-Methylphenol	108-39-4	<i>m</i> -Cresol; <i>meta</i> -cresol
4-Methylphenol	106-44-5	<i>p</i> -Cresol; <i>para</i> -cresol
<b>Halogenated organics</b>		
1,1,2 Trichloroethane	79-00-5	1,1,2-TCA; ethane trichloride; $\beta$ -trichloroethane; vinyl trichloride
1,1-Dichloroethane	75-34-3	1,1-DCA; $\alpha,\alpha$ -dichloroethane; CFC-150a
1,1-Dichloroethene	75-35-4	1,1-DCE; 1,1-dichloroethylene; vinylidene chloride
1,2-Dichloropropane	78-87-5	1,2-DCP; propylene dichloride
2-Chloronaphthalene	91-58-7	2-Naphthyl chloride; $\beta$ -Chloronaphthalene
Bromobenzene	108-86-1	Phenyl bromide; bromobenzol; monobromobenzene
Bromodichloromethane	75-27-4	Dichlorobromomethane
Bromoform	75-25-2	Methyl tribromide; tribromomethane
Chloroethane	75-00-3	Monochloroethane; ethyl chloride; ethylene chloride
Chloromethane	74-87-3	Methyl chloride; Freon-40; monochloromethane
<i>cis</i> -1,2 Dichloroethene	156-59-2	<i>cis</i> -1,2-DCE; <i>cis</i> -1,2-dichloroethylene
<i>trans</i> -1,2 Dichloroethene	156-60-5	<i>trans</i> -1,2-DCE; <i>trans</i> -1,2-dichloroethylene
Dichloromethane	75-09-2	DCM; methylene chloride; methylene dichloride; Freon-30
Hexachloroethane	67-72-1	PCA; perchloroethane; carbon hexachloride; hexachloroethylene
<b>Phthalates</b>		
Bis (2-ethylhexyl) phthalate	117-81-7	DEHP; BEHP; di-2-ethyl hexyl phthalate
Butyl benzyl phthalate	85-68-7	BBP; <i>n</i> -butyl benzyl phthalate; benzyl butyl phthalate; BBzP
Diethyl Phthalate	84-66-2	DEP; ethyl phthalate; 1,2-benzenedicarboxylic acid diethyl ester
Di- <i>n</i> -butyl phthalate	84-74-2	DBP; <i>n</i> -butyl phthalate; 1,2-benzenedicarboxylic acid dibutyl ester
Di- <i>n</i> -octyl phthalate	117-84-0	1,2-Benzenedicarboxylic acid, dioctyl ester
<b>Other Organics</b>		
Biphenyl	92-52-4	diphenyl; phenyl benzene; 1,1-biphenyl; lemonene
2,4-Dinitrotoluene	121-14-2	2,4-DNT
2,6-Dinitrotoluene	606-20-2	2,6-DNT
Tributyl tin oxide	56-35-9	TBTO; bis(tri- <i>n</i> -butyltin)oxide
Methyl <i>tert</i> -butyl ether	1634-04-4	MTBE; <i>tert</i> -butyl methyl ether; methyl <i>tertiary</i> -butyl ether

GAC have been derived for 4 generic land-uses; residential with consumption of homegrown produce, residential without consumption of homegrown produce, allotments and commercial land-use. The generic assumptions used for deriving the GAC for each of these land-uses are described in detail in the Environment Agency of England and Wales SR3 report (2009a).

Each land-use scenario has had GAC produced for 3 soil organic matter (SOM) contents; 1%, 2.5% and 6%. This range in SOM is considered a reasonable representation of the majority of soils within the UK. Note that due to limitations in time and scope of the project plant uptake factors were not derived for the metals (see Section 3.4) and therefore the metals GAC have only been produced for the residential without consumption of homegrown produce and commercial land-uses.

Physico-chemical data were collated for a further 9 organic contaminants as listed in Table 2.2. However, there were insufficient toxicological data available to derive health criteria values (HCV) that were acceptable to the entire group of risk assessors and consequently GAC are not presented for these contaminants. This is not to say that there are insufficient data to assess the risk from these compounds on a site specific basis but rather that the uncertainties involved prevent the derivation of industry agreed GAC for general use on all sites within the UK.

Data collated for the 44 contaminants assessed are provided in Appendix B.

Table 2.2: Additional contaminants researched but with insufficient data to derive EIC/AGS/CL:AIRE GAC

Substance	CAS	Synonyms
1-Methylnaphthalene	90-12-0	$\alpha$ -Methylnaphthalene
2-Methylnaphthalene	91-57-6	$\beta$ -Methylnaphthalene
1,3,5-Trimethylbenzene	108-67-8	Mesitylene; sym-trimethylbenzene
Carbazole	86-74-8	9-Azofluorene; dibenzopyrrole; diphenylenimine; diphenylenemide
Dimethyl phthalate	131-11-3	Dimethyl 1,2-benzenecarboxylate
Isopropyltoluene	99-87-6	4-Isopropyltoluene; p-Isopropyltoluene; 1-methyl-4-propan-2-ylbenzene; p-methylcumene; cymene
<i>n</i> Butylbenzene	104-51-8	1-Butylbenzene; 1-phenylbutane
<i>sec</i> Butylbenzene	135-98-8	2-Butylbenzene; 2-phenylbutane
<i>tert</i> Butylbenzene	98-06-6	Pseudobutylbenzene; dimethylethylbenzene; trimethylphenylmethane

## 2.2 Use of EIC/AGS/CL:AIRE GAC

The GAC have been derived in general accordance with the CLEA framework documents (see Section 3) and are intended to be used in the same way as the SGV. Guidance on the use of SGV is provided in the Environment Agency of England and Wales report entitled "Using Soil Guideline Values" (Environment Agency, 2009a) and although intended for the use of SGV, this guidance is also highly relevant to the use of the EIC/AGS/CL:AIRE GAC. The reader should therefore familiarise themselves with this guidance before using the GAC. The reader is also recommended to familiarise themselves with the SR2, SR3 and SR7 CLEA methodology framework documents (Environment Agency, 2009b, 2009c and 2008), the CLEA software handbook (Environment Agency, 2009d) and the Environment Agency of England and Wales CLR11 technical framework document for assessing and managing risks from land contamination (Environment Agency, 2004).

## 2.2.1 What the EIC/AGS/CL:AIRE GAC are

The Environment Agency of England and Wales guidance describes what SGV are and are not. These definitions apply equally to the EIC/AGS/CL:AIRE GAC and are summarised in Box 1.

### Box 1. What the EIC/AGS/CL:AIRE GAC are/are not

#### Definition of what EIC/AGS/CL:AIRE GAC are:

- They are scientifically based screening criteria that have been derived using the CLEA model (v1.06) in general<sup>2</sup> accordance with the CLEA framework;
- They can be used as a starting point for evaluating long-term risks to human health from chemicals in soil; and
- They provide an indication of the chemical concentration in soil below which the long-term human health risks for site occupants (for various generic land-use scenarios) are considered to be tolerable or minimal
- They are screening criteria to determine the need for further investigations and the need for a DQRA.

#### Definition of what EIC/AGS/CL:AIRE GAC are NOT:

- They do not represent the "trigger" for unacceptable intake, i.e. exceedence of the GAC does not necessarily imply *significant possibility of significant harm* (SPOSH);
- They do not cover other types of risk to humans such as fire, suffocation or explosion, risks from chemicals in groundwater or ground gas or short term and acute exposures;
- They cannot be used to evaluate risks to construction workers or non-human receptors; and
- They are not explicitly derived to define remediation standards.

## 2.2.2 How the EIC/AGS/CL:AIRE GAC should be used

Like the SGV, the EIC/AGS/CL:AIRE GAC have been derived based on generic conceptual site models for a number of land-uses and making generic assumptions about receptor type and behaviour and building and soil properties. These generic assumptions must be considered in the context of the conceptual site model to determine whether the GAC are an appropriate tool for assessing risks at the site under consideration. The practitioner should familiarise themselves with the suite of CLEA framework documents in order to understand these assumptions and the methodology used for deriving GAC. In particular, the assessor should consider the following:

- Are there potential pollutant linkages present that the GAC do not consider, e.g. risk to workers in excavations, inhalation of vapours generated from contaminants in groundwater, diffusion of contaminants through drinking water pipes? The presence of such pollutant linkages does not preclude the use of GAC, but the assessor should recognise that the use of GAC alone will not assess all the potential risks at the site;

<sup>2</sup> Unlike the SGVs the EIC/AGS/CL:AIRE GAC are not in strict accordance with the CLEA framework. For example, the CLEA SR2 document recommends the use of an expert toxicologist to review the health criteria from expert review groups and to challenge these criteria where appropriate. Although the EIC/AGS/CL:AIRE GAC project volunteers were all experienced human health risk assessors none were qualified toxicologists and thus the HCV have been derived on the basis of available health criteria and guidance provided in the SR2 document.

- Are all the exposure pathways used for the derivation of GAC appropriate at the site? For example, the presence of hard-standing may prevent the generation of dusts and/or direct contact with soil;
- Are the generic parameter values used for the derivation of GAC reasonable for the site? For example, the residential GAC may not be protective for a house with a large garden used almost exclusively for the cultivation of homegrown fruit and vegetables.

Like the SGV, the EIC/AGS/CL:AIRE GAC represent minimal or tolerable risk. As such, they present useful screening criteria for the assessment of risks. Care should be taken if adopting these values for other purposes, such as acceptance criteria for imported topsoil. Although the GAC may prove convenient screening criteria for this purpose it should always be recognised that they are based on generic assumptions and parameter values and that the development of site-specific assessment criteria protective of human health may be more appropriate at some sites.

### 2.2.3 Consultation

One key difference between the EIC/AGS/CL:AIRE GAC and the SGV relates to the degree of consultation undertaken in their derivation / publication. The SGV (and associated HCV) have been derived by the Environment Agency of England and Wales in consultation with other Government departments and agencies, including the Food Standards Agency and the Health Protection Agency. The EIC/AGS/CL:AIRE GAC have not been subject to this level of consultation and unlike the SGV are not endorsed by DEFRA, the HPA or the Environment Agency of England and Wales.

Nevertheless, the EIC/AGS/CL:AIRE GAC do carry a level of authority for the following reasons:

- They have been derived using the CLEA model (v 1.06) in general accordance with the CLEA framework of guidance documents;
- They have been researched and agreed on by a group of experienced human health risk assessors from 26 EIC and AGS member companies;
- They have been subject to a high degree of internal review (see Sections 3.1.2 and 3.1.3); and
- Various external authoritative bodies were invited to read and comment on a pre-publication version of the EIC/AGS/CL:AIRE GAC report (see Section 3.1.3). Comments were received from the Environment Agency of England and Wales, the Royal Environmental Health Institute of Scotland (REHIS), Environmental Protection UK, the Northern Ireland Environment Agency, the Chartered Institute of Environmental Health (CIEH) and the Scottish Environment Protection Agency (SEPA). These comments mostly related to the overall approach and wording of the main text and included recommendations for improving the clarity of the report. These comments have all been considered and with few exceptions addressed in the final version of the report. All of the comments significant to the derivation or application of the GAC have been addressed. Comments not addressed related to style and/or presentation of report. It is noteworthy that the Environment Agency of England and Wales commented that the approach described for derivation of the EIC/AGS/CL:AIRE GAC appeared to be broadly consistent with the CLEA guidance with some exceptions (which are highlighted in this report).

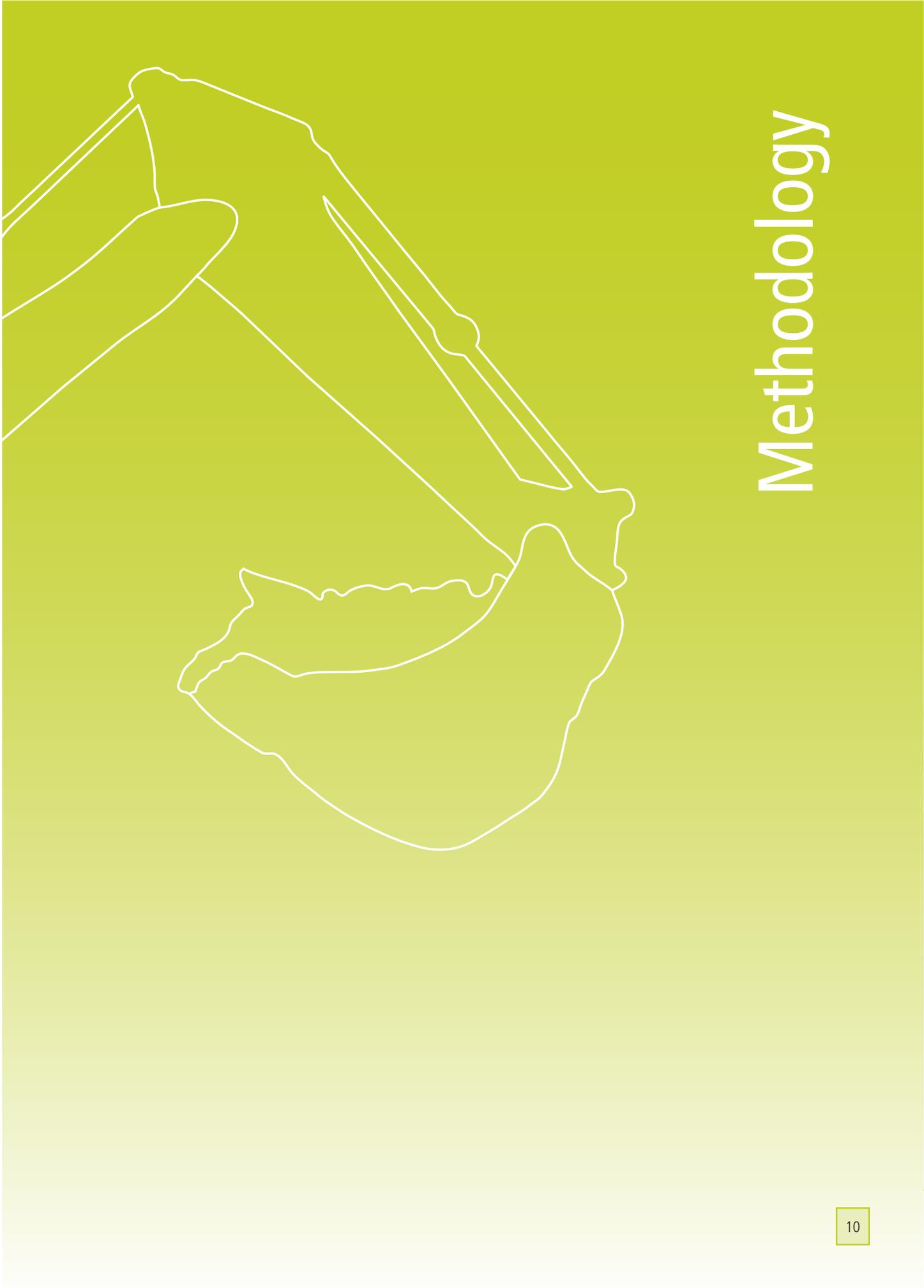
It should be noted that none of the external authoritative bodies have carried out a detailed technical review of any of the recommended physico-chemical and toxicological properties or GAC values presented in this report.

As a result it is anticipated that these GAC will become widely accepted and draw authority in the UK as appropriate screening criteria to aid the assessment of risks to human health from soil contamination in the UK.

#### 2.2.4 Other considerations when using the EIC/AGS/CL:AIRE or other GAC

There are a number of other aspects that must be considered regarding the EIC/AGS/CL:AIRE GAC :

- Alternative GAC. The selection of parameter values was conducted in general accordance with the CLEA framework and in particular the Environment Agency of England and Wales SR2 (Environment Agency, 2009c) and SR7 (Environment Agency, 2008) reports. The adherence to protocol increases consistency in parameter value choice but does not remove the necessity for professional judgement. Others may disagree with the professional judgements made and so this report attempts to be as transparent as possible to allow others to utilise the data but make their own professional judgement on parameter value selection. Importantly, differences in professional opinion over parameter value selection can mean that two alternative GAC for one contaminant are equally valid. Thus the availability of EIC/AGS/CL:AIRE GAC does not invalidate other GAC produced and used by other organisations in the UK for the same contaminants, provided that the assumptions used for their derivation are clearly set out to enable an assessor to understand the differences and to make their own decision on which is appropriate in the specific circumstances.
- Lifetime of EIC/AGS/CL:AIRE GAC . The EIC/AGS/CL:AIRE GAC have been derived using the latest CLEA model (v1.06) and framework guidance available at the time of writing. The validity of the GAC may need to be re-considered if the CLEA model or guidance documents are revised in the future. This also applies to the data from which the contaminant properties have been derived for the EIC/AGS/CL:AIRE GAC . For example, the health criteria values (HCV) used for deriving the GAC are based on authoritative toxicological reviews available when the EIC research was conducted in spring/summer 2009. New toxicological studies or the revised interpretation of existing studies could mean that some of the HCV used will become outdated. Assessors should be aware of this possibility and assess the suitability of the GAC should this occur. Additionally, should an SGV report for a substance contained in this report be published by the Environment Agency of England and Wales, the SGV would take precedence over the relevant GAC.



# Methodology

## 3 Methodology

### 3.1 Overview of Process

The project was conducted over a number of phases detailed below.

#### 3.1.1 Phase 1: Project scoping

A scoping study was conducted in December 2008 to assess the level of effort required to produce GAC compliant with the current CLEA methodology and to enable realistic goals and timescales to be set for the project. Contributing organisations were asked to indicate the contaminants for which they had previously derived GAC. This resulted in a list of a possible 150+ substances. These were ranked according to the number of consultants that had derived GAC for each substance and the top 44 contaminants were selected. In preparing the priority list, the project team conferred with both the Environment Agency of England and Wales and LQM/CIEH to ensure that there was no duplication of effort with the forthcoming publication of SGV or LQM/CIEH GAC.

A workshop was held in February 2009 for all participating organisations to finalise the list of contaminants, agree procedures for the collation of data and peer review, allocate tasks and set the project schedule.

#### 3.1.2 Phase 2: Data compilation and peer review

Phase 2 involved the collation of data, selection of appropriate contaminant specific parameter values for use in the CLEA model and peer review. To ensure that this process was efficient and transparent as possible, a series of proformas were designed to capture the relevant data and justify why particular parameter values had been chosen. This ensured that the process of collecting data and selecting parameter values was consistent for all 44 contaminants reviewed.

Each contaminant had three proformas as described in Table 3.1. The finalised proformas for all 44 contaminants are provided in Appendix B. Further details of the contents of these proformas are provided in Sections 3.2, 3.3 and 3.4.

Table 3.1: Proformas used for data collation and parameter value selection

Proforma	Description
Health Criteria Values	Used to present pertinent toxicological information from authoritative bodies. Proforma also shows recommended health criteria values and justification for the choice of values.
Mean Daily Intakes	Used to present pertinent background exposure information. Proforma also shows recommended mean daily intake values and justification for the choice of values.
Physico-chemical Properties	Used to present relevant physico-chemical information from authoritative data sources. Proforma also shows recommended physico-chemical parameter values and justification for the choice of values.

Each of the 26 volunteering organisations was generally allocated 3 to 4 contaminants to review (although some reviewed up to 6 contaminants). Peer review partners were assigned so that each group of contaminants was allocated to two volunteering organisations. This ensured that each contaminant was independently researched by a pair of volunteers.

The volunteers then had a period of 2 months to collate data for their allocated contaminants and produce the proformas with recommended CLEA input values. Proformas were then swapped between pairs, reviewed and an attempt made to resolve any discrepancies or differences in opinion. The pairs of proformas were then distilled into one unified set of proformas for each contaminant.

A second workshop was held in May 2009 to resolve any remaining issues from the data collation and peer review process. Protocols for selection of recommended CLEA input parameters were finalised at this workshop.

### 3.1.3 Phase 3: Proforma finalisation, production of GAC and preparation of report

Phase 3 involved the second tier of technical review, derivation of GAC and report production. The second tier of review comprised two review panels, each consisting of 5 or 6 volunteers. One panel reviewed the health criteria value and mean daily intake proformas and one reviewed the physico-chemical proformas. The panel reviews took place in a series of one day workshops and were designed to ensure that a consistent approach had been taken for the selection of recommended parameter values. Modifications were made to the proformas as necessary and the recommended values used to derive the EIC/AGS/CL:AIRE GAC .

The GAC were derived independently by three volunteers and the results were compared for consistency. The finalised proformas and GAC were then collated in a pre-publication report. This was issued to the organisations listed in Box 2, who were asked to provide comments within a period of four weeks. In addition, representatives from the EIC Contaminated Land Working Group, CL:AIRE and AGS, who were not involved in the collation of data, were asked to review and provide comment on the report.

Box 2: External organisations invited to comment on pre-publication version of report	
<ul style="list-style-type: none"> <li>Environment Agency of England and Wales</li> <li>Health Protection Agency</li> <li>Royal Environmental Health Institute of Scotland</li> <li>Environmental Protection UK</li> <li>Scotland and Northern Ireland Forum for Environmental Research</li> </ul>	<ul style="list-style-type: none"> <li>Chartered Institute of Environmental Health</li> <li>Northern Ireland Environment Agency</li> <li>Scottish Environment Protection Agency</li> <li>Soil and Groundwater Technology Association</li> </ul>

As discussed in Section 2.2.3 comments were received from six organisations. The comments related to the overall approach and the content of the text section of this report. All of the comments significant to the derivation or application of the GAC have been addressed. Comments not addressed related to style and/or presentation of report. The external organisations did not (and were not expected to) carry out a detailed technical review of the parameter values or GAC presented in this report.

## 3.2 Derivation of Health Criteria Values

The procedures for collation and choice of health criteria values (HCV) were in general accordance with the principles set out in SR2, Human Health Toxicological Assessment of Contaminants in Soil (Environment Agency, 2009c). One exception to the recommendations in SR2 concerns the use of expert toxicologists. SR2 recommends the use of an expert toxicologist in the derivation of HCV to review the health criteria from expert review groups and to challenge these criteria where appropriate. Although the EIC/AGS/CL:AIRE GAC project volunteers were all experienced human health risk assessors none were qualified toxicologists and thus the HCV have been derived on the basis of

available health criteria derived by expert review groups and guidance provided in the SR2 document for identifying which of these criteria are most appropriate for the derivation of HCV.

All 33 sources listed in Appendix A of the SR2 report were consulted and relevant data for each contaminant were summarised on the contaminant proformas. Note that sources that held no data relevant to the substance have been removed from the proforma to reduce the overall length of Appendix B. Other sources, not listed in the SR2 report were also consulted, including:

- US Environment Protection Agency (US EPA) Provisional Peer Reviewed Target Values (PPRTV), available by request from the EPA Superfund Health Risk Technical Support Center;
- US Oak Ridge Risk Assessment Information System (RAIS), available on the web at [http://rais.ornl.gov/cgi-bin/tools/TOX\\_search?select=chem](http://rais.ornl.gov/cgi-bin/tools/TOX_search?select=chem)
- US Army Corps of Engineers, available on the web at <http://el.erd.c.usace.army.mil/arams/>
- Texas Commission on Environmental Quality, available on the web at <http://www.tceq.state.tx.us/remediation>

US EPA PPRTV reports were obtained for all contaminants where available. The latter three sources lacked provenance of data, and were generally only consulted if data from the other sources were lacking.

The HCV proformas are organised into five sections:

1. A header section showing whether the HCV are based on threshold or non-threshold toxicity and which exposure routes the HCV are applied to for the derivation of GAC;
2. A section summarising information from the authoritative sources on threshold health effects via oral exposure and giving the recommended Tolerable Daily Intake (TDI) for oral exposure for input to the CLEA model;
3. A section summarising information from the authoritative sources on threshold health effects via inhalation exposure and giving the recommended TDI for inhalation exposure for input to the CLEA model;
4. A section summarising information from the authoritative sources on non-threshold health effects via oral exposure and giving the recommended index dose (ID) for oral exposure for input to the CLEA model; and
5. A section summarising information from the authoritative sources on non-threshold health effects via inhalation exposure and giving the recommended ID for inhalation exposure for input to the CLEA model.

The relevant information from each authoritative source is organised into columns. This information includes the toxicological benchmark adopted by that authoritative body (if any) and the provenance of that benchmark, including uncertainty factors, details of the study (or studies) that the benchmark is based on (i.e., study type, duration, species, reference etc.) and whether the benchmark is based on a no-observed adverse effect level (NOAEL) or lowest-observed adverse effect level (LOAEL).

A summary of the justification for selection of HCV is provided next to each of the recommended HCV on the contaminant specific proformas. The overall approach used in the selection of recommended HCV are summarised in the following sections.

### 3.2.1 Threshold and non-threshold behaviour

The data sources were reviewed for information on the threshold and non-threshold behaviour of contaminants. Generally, the decision to consider a contaminant as non-threshold was based on the classification given by the International Agency for Research on Cancer (IARC), if available. Contaminants rated with an IARC classification of Group 3 (not classifiable as to its carcinogenicity to humans) or less were considered as threshold substances

unless there was more recent strong evidence to suggest that treatment as a non-threshold substance would be appropriate. In some cases, even if there was reasonable evidence of human carcinogenicity, there was insufficient dose-response data on non-threshold effects to derive an index dose and the HCV were therefore based on threshold effects alone.

### 3.2.2 Selection of recommended TDIs and IDs

As far as possible, SR2 guidance on the selection of TDIs and IDs has been followed. As previously discussed, the SR2 guidance for derivation of HCV recommends the use of an expert toxicologist. This toxicologist should be able to evaluate the merits of alternative health criteria and, if required, derive HCV *de novo* (i.e. derive HCV directly from toxicological data). As discussed, none of the EIC/AGS/CL:AIRE GAC project volunteers were qualified toxicologists and therefore no attempt has been made to derive HCV *de novo*. Rather, TDIs and IDs were selected from the collated health criteria derived by national and international expert review groups. It should also be noted that the HCV for contaminants with SGV have in general been derived from existing health criteria from expert review groups as opposed to *de novo*. To ensure that a consistent approach was followed, the following protocol was derived and used for the derivation of HCV:

- TDIs or IDs were not recommended if there were insufficient data with sufficient details on provenance. For example, for some contaminants, the only health criteria available were reference doses (RfD), reference concentrations (RfC) or carcinogenic slope factors given in web-based databases such as RAIS. These databases did not provide sufficient supporting data (such as details on the study that the health criteria was based on) to have confidence that the health criterion was suitable for derivation of an EIC/AGS/CL:AIRE GAC. In these cases, no TDI or ID were recommended.
- Information sources labelled as draft with “do not cite or quote” have not been used to derive HCV, but are referred to in the proformas for information.
- Occupational exposure levels (OEL) have not been used to derive HCV, but OEL data are reported in the proformas for information.
- Insufficient data on dermal exposure toxicity were identified to enable the derivation of HCV for dermal exposure. In accordance with the Environment Agency of England and Wales SR2 document, in the absence of data on dermal toxicity the HCV for oral exposure (where available) have been used for assessing dermal exposure in the CLEA model. For contaminants where no oral HCV has been derived, route-to-route extrapolation from inhalation data has been considered as discussed below.
- Route-to-route extrapolation has been considered for substances where an HCV has been derived for only one route of exposure. The SR2 document cites IGHRC (2006) for guidance on the use of route-to-route extrapolation. Route-to-route extrapolation may under- (or over-) estimate toxicity due to differences in absorption, metabolism and mode of action between routes of exposure. Oral to inhalation extrapolation is only recommended when: (a) the critical toxicological effect is systemic (rather than at the initial site of contact); (b) first pass metabolism (i.e. metabolism in the liver) and/or metabolism in the gut are not significant; and (c) there is sufficient information on the relative acute toxicity and/or bioavailability between routes of exposure. The IGHRC note that inhalation to oral extrapolation is less likely to underestimate toxicity because absorption in the gastrointestinal tract is typically lower than in the lungs.

Of the 44 substances researched 19 had a recommended HCV<sub>oral</sub> but no HCV<sub>inhal</sub> and 3 had a recommended HCV<sub>inhal</sub> but no HCV<sub>oral</sub>. An initial review revealed that there were unlikely to be sufficient data to satisfy all three conditions for the 19 compounds with an HCV<sub>oral</sub> and no HCV<sub>inhal</sub>.

Despite the lack of data the decision was taken to use route-to-route extrapolation unless there was evidence to suggest that this was not appropriate. The alternative would have been to not derive GAC for these compounds. This option was considered less useful than having a set of GAC for compounds where there remained some uncertainty in the inhalation HCV used to derive them.

There were two cases where route-to-route extrapolation was considered inappropriate: 1-methylnaphthalene and 2-methylnaphthalene, both of which have an  $HCV_{oral}$  but no  $HCV_{inhal}$ . There was evidence to suggest that the toxicity of these compounds via inhalation was likely to be significantly greater than their toxicity via ingestion and therefore use of the  $HCV_{oral}$  may have resulted in GAC that were unprotective.

- Where alternative health criteria were available from different authoritative sources then priority was given to the most recent expert reviews, provided these had considered all available data. Preference was also given to longer term studies. Where there was no clear case for selection of a particular HCV, priority was given to the most conservative.
- Three contaminants were considered as non-threshold substances; 1-methylnaphthalene, bromodichloromethane and carbazole. There were insufficient data to derive an ID for carbazole. Dose-response data with reported 95<sup>th</sup> percentile lower confidence limit benchmark dose levels (BMDL10) derived from animal experiments involving oral exposure were available for 1-methylnaphthalene and bromodichloromethane and these were used to derive the  $ID_{oral}$  for each contaminant in accordance with the methodology given in the Environment Agency of England and Wales SR2 report.
- Reference concentrations (RfC) have been converted to inhalation HCV in accordance with the Environment Agency of England and Wales SR2 guidance, i.e. by multiplying by 20 m<sup>3</sup> of air inhaled per day and dividing by 70 kg standard body mass.

### 3.3 Selection of Mean Daily Intakes

The procedures for collation and choice of mean daily intake (MDI) were in general accordance with the principles set out in the Environment Agency of England and Wales SR2 document. As with the HCV, all 33 sources listed in Appendix A of the SR2 report were consulted and relevant data for each contaminant were summarised on the contaminant proforma. Again, sources that held no data relevant to the substance have been removed from the proforma to reduce the overall length of Appendix B. Assumptions used in the selection of recommended MDI are summarised below:

- MDI have been based on available relevant data. Data from near point sources were not considered relevant and have not been used for the derivation of MDI.
- Preference has been given to data on likely average exposure to the UK population. If no UK data were available preference was given to average exposure from other countries. Where only maximum values were reported, but did not relate to point sources, then these were used as a conservative estimate of MDI.
- Where suitable data were available from more than one information source and there was no obvious preference for one of these sources then the most conservative (highest) value was chosen as the basis of the MDI.
- If no data were available and the literature suggests the exposure is likely to be negligible, the MDI has been set to zero, in line with SR2.

- In accordance with the Environment Agency of England and Wales SR2 document air concentrations (mass per m<sup>3</sup>) have been converted to MDI<sub>inhal</sub> by multiplying by an assumed 20 m<sup>3</sup> of air inhaled per day. Drinking water concentrations (mass per litre) have been converted to MDI<sub>oral</sub> by multiplying by an assumed 2 litres of water ingested per day.

### 3.4 Derivation of Physico-Chemical Parameters

A knowledge of the physico-chemical behaviour of a potential chemical contaminant is necessary in order to successfully model its fate in the environment. In order to produce GAC within the CLEA v 1.06 model a number of physico-chemical properties of a contaminant must be known. Some of these properties can be directly measured in the laboratory while others are estimated from knowledge of other physico-chemical parameters or the structure of the molecule.

All of the physico-chemical parameters for the organic substances required for the CLEA v1.06 model have been obtained in general accordance with the principles set out in SR7, Compilation of Data for Priority Organic Pollutants for Derivation of Soil Guideline Values (Environment Agency, 2008). The same 9 literature reference sources set out in Table 1.3 of SR7 were reviewed for each substance and all relevant data were recorded on the proformas by each volunteer.

The procedures outlined in SR7 were also used to obtain physico-chemical parameters required for the 3 metals investigated, though the number of properties required are significantly less than for the organics. Note that, as discussed below, plant uptake has not been modelled for the 3 metals. These metals are not volatile and therefore the only physico-chemical property required for the metals is the dermal absorption factor. Literature derived values of solubility and soil-water partition coefficient are provided in the proformas but no recommended single values have been derived as these parameters were not required for the GAC produced.

The proformas issued to all volunteers also included embedded routines to estimate physico-chemical properties where no literature values were available and to correct properties to 10°C where appropriate. All calculations included in the proforma are those recommended in SR7. Calculations used in the proformas were peer reviewed and quality assurance tested prior to use in this project by volunteers.

Table 3.2 lists the physico-chemical parameters required for the CLEA v1.06 model. Some of the parameters listed in this table are required in an indirect capacity; they are used to aid in the calculation/estimation of other properties that are directly used within the model. Additionally, some of the chemical parameters can be obtained from literature references while others require estimation by use of accepted methods.

Table 3.2: Summary of Required Physico-Chemical Parameters

Property	Units	Symbol	Comment
Molecular Mass	g/mol	MW	Used both directly within the CLEA model and to estimate other properties.
Henry's Law Constant	Pa · m <sup>3</sup> /mol	H	Temperature dependent relationship of the partial pressure of a gas above a liquid which the gas is dissolved in. Used to estimate the K <sub>aw</sub> in the absence of measured solubility data at the ambient soil temperature (i.e. 10°C)
Solubility	mg/L	S	A temperature dependent expression of the mass of a substance that will dissolve completely in water - used directly within the CLEA model. Solubility data, if available at ambient soil temperature (10°C), is also used to estimate K <sub>aw</sub> via the direct calculation method.

Property	Units	Symbol	Comment
Boiling Point	K	$T_b$	The temperature at which the vapour pressure of a liquid is equal to the atmospheric pressure; the normal boiling point is measured when the atmospheric pressure is equal to 1 atm. $T_b$ is used to estimate a number of properties used within the CLEA model.
Melting Point	K	$T_m$	The temperature which a solid substance changes state to a liquid; the normal melting point is measured when the atmospheric pressure is equal to 1 atm. $T_m$ is used to estimate the vapour pressure of a substance.
Log Octanol - Water Partition Coefficient	-	$\log K_{ow}$	A measure of a substance's preference to dissolve in an organic solvent or water. The $\log K_{ow}$ is used both directly within the CLEA model and to estimate the organic carbon - water partition coefficient.
Molar Volume	$\text{cm}^3/\text{mol}$	$V_B$	The volume occupied by one mole of a substance at a given temperature and pressure. $V_B$ is used to estimate the diffusion coefficients in air and water.
Enthalpy of Vaporisation	$\text{J}/\text{mol}$	$\Delta H_{vap}$	The energy required to convert one mole of a substance from a liquid to a gas at a given temperature and pressure. $\Delta H_{vap}$ is used both directly with the CLEA model and to estimate P and $K_{aw}$ (using the Clapeyron relationship from H at 25°C). $\Delta H_{vap}$ has been estimated using the modified Klein method.
Critical Temperature	K	$T_c$	The temperature and pressure above which the liquid and gas phases are indistinguishable. Used to estimate $\Delta H_{vap}$ and $K_{aw}$ (using the Clapeyron relationship from H at 25°C). Critical points have been estimated using the Lydersen method which accounts for structural features of the substance.
Critical Pressure	atm	$P_c$	
Air - Water Partition Coefficient	$\text{cm}^3/\text{cm}^3$	$K_{aw}$	The constant of proportionality describing the partitioning of a substance between air and water used directly within the CLEA model. If solubility data are available at the ambient soil temperature (i.e. 10°C), $K_{aw}$ has been estimated using the direct calculation method; otherwise it has been estimated via the Clapeyron relationship from H at a known reference temperature
Vapour Pressure	Pa	P	The pressure of the gas of a substance in equilibrium with the substance as a solid/liquid at a given temperature. P is used both directly within the CLEA model and to estimate $K_{aw}$ via the direct calculation method. P, at ambient soil temperature (i.e. 10°C), has been estimated using the Grain and Watson method.
Diffusion Coefficient in Air	$\text{m}^2/\text{s}$	$D_a$	A measure of the diffusion of a molecule of a substance in air used directly in the CLEA model. $D_a$ has been estimated using the Wilke and Lee method.
Diffusion Coefficient in Water	$\text{m}^2/\text{s}$	$D_w$	A measure of the diffusion of a molecule of a substance in water used directly in the CLEA model. $D_w$ has been estimated using the Hayduk and Laudie method.
Log Organic Carbon-Water Partition Coefficient	$\log(\text{cm}^3/\text{g})$	$\log K_{oc}$	A partition coefficient that expresses the tendency of a compound to be absorbed onto the organic carbon within the soil as opposed to being dissolved in the soil water. The $\log K_{oc}$ is used directly within the CLEA model and is estimated from $K_{ow}$ dependent on the class of the organic compound using the Forman, Guldbery and Thodos Approximation.

Property	Units	Symbol	Comment
Soil Water Partition Coefficient	cm <sup>3</sup> /g	K <sub>d</sub>	A coefficient relating to the partitioning of a substance between the solid and aqueous phases used directly within the CLEA model. Literature values required for inorganic substances for the plant uptake pathways, while the model estimates values for organic substances based on K <sub>oc</sub> and the soil organic matter content.
Dermal Absorption Fraction	-	ABS <sub>d</sub>	A measure of the ability of a substance to desorb from soil adhered to the skin and adsorb across the skin into the bloodstream. In the absence of literature values SR3 recommends the use of generic default ABS <sub>d</sub> values; default values for organics and inorganics are 0.1 and 0 respectively.

Selection of adopted values for each physico-chemical parameter was undertaken in general accordance with the methodology set out in Section 1.2.2 (Review methodology), summarised in Table 1.4 of SR7. Ambiguities in the Environment Agency of England and Wales method were interpreted by the Physico-Chemical Review Panel so that a consistent approach has been used across all substances included in this report.

Proformas are available for each substance studied and are presented within Appendix B of this report. Each proforma includes all of the individual data obtained for each property from each of the nine literature references reviewed. Either the geomean or average of all values from each reference (in accordance with SR7) was also calculated; these values are also included on the attached proformas. The adopted value for each property, along with the selection rationale can also be found on the proforma.

The aims of the physico-chemical data research were to follow the best available guidance on physico-chemical selection as closely as possible while at the same time being transparent in the methods used. All of the values found during the literature review process have been included on the attached substance specific proformas. The adopted values, with included rationale for selection, are based on the Review Panel's interpretation of the guidance available in SR7. However, all of the data have been included on the proformas to enable the risk assessor using these values to understand the range of values recorded for each individual parameter as well as choose a different value that in their professional judgement is more appropriate for the specific circumstances of their assessment.

Where data were reported in the literature for a physico-chemical property at more than one reference temperature (e.g. solubility), data reported at the temperature closest to the default ambient soil temperature used in the CLEA model (i.e. 10°C) were recorded on the proforma.

Plant concentration factors for organic contaminants are estimated within the CLEA v1.06 model by the empirical methods outlined within Chapter 7 of SR3, Updated Technical Background to the CLEA model (Environment Agency, 2009b). Due to limitations in volunteered time, it was considered beyond the scope of this project to undertake appropriate research to derive plant concentration factors for the 3 inorganic substances covered (i.e. antimony, barium and molybdenum). Where plant concentration factors were found for these inorganic substances they have been recorded on their proformas for information purposes only. Plant concentration factors have not been recommended for these substances and GAC have not been produced for the generic land uses that include the plant uptake pathway (i.e. residential with consumption of homegrown produce or allotments).

The dermal absorption factors recommended in SR3, have been adopted in the derivation of GAC. A default value of zero has been used for the metals and 0.1 has been used for the organics with the exception of 1-methylnaphthalene, 2-methylnaphthalene, 2,4-dinitrotoluene and 2,6-dinitrotoluene, which are listed in Table 8.2 of SR3 and have values of 0.13, 0.13, 0.102 and 0.099, respectively.

### 3.5 Derivation of GAC

GAC were derived using the CLEA model v1.06. The recommended values from the proformas were transposed to the contaminant database in the CLEA model. A copy of the contaminant database used to derive the GAC is provided as a freely downloadable spreadsheet with this report. A summary of the contaminant database is provided in Appendix A. GAC were produced for those contaminants with recommended values for all the required parameters. Note that, with the exception of di-*n*-butyl phthalate (which has evidence of localised toxicological effects in the upper respiratory tract – see Section 3.7) the critical toxicity of all compounds is expected to be systemic. For this reason, where HCV were available for both the inhalation and oral routes of exposure, the combined GAC have been reported.

The derived GAC and exposure contributions for each pathway calculated by CLEA v1.06 are presented in Tables 4.1a to 4.4e. Note that the GAC have been rounded to two significant figures. The pathway exposure contributions have been reported to one decimal place and are intended to aid the risk assessor in determining the appropriateness of the GAC for the site-specific conceptual site model.

Table 4.1a presents the GAC for the metals. As discussed in Section 3.4, it was considered beyond the scope of the project to collate and review plant concentration factors for the metals and therefore GAC have only been produced for land-uses that do not include plant uptake, i.e. the residential without homegrown produce and commercial land-uses. Note that the derived GAC for metals are not dependent on SOM.

Tables 4.2a, 4.3a and 4.4a present the GAC for 32 organic contaminants assuming 1%, 2.5% and 6% SOM, respectively. These tables also present the estimated soil saturation concentration<sup>3</sup> for each contaminant (rounded to three significant figures). As discussed in the Environment Agency of England and Wales SR2 report, soil concentrations exceeding soil saturation may indicate the presence of non-aqueous phase liquid (NAPL) and this should be considered when assessing the risks to human health. The presence of NAPL could pose additional risks to human health that are not accounted for in the GAC, such as the inhalation of vapours arising from NAPL sources and direct contact with NAPL. Odours arising from NAPL may also be cause for concern.

As discussed in Section 3.2, HCV were not always available for both the oral and inhalation pathways. Where this was the case and where considered appropriate the use of route-to-route extrapolation, whereby the HCV for the oral route is applied to inhalation exposures and vice versa, has been adopted. This has been done in the CLEA model by selecting “Y,Y,Y” for the recommended HCV in the contaminant database such that the estimated average daily exposures (including MDIs) for the oral, dermal and inhalation pathways are compared to this HCV to derive the GAC.

<sup>3</sup> The soil saturation concentration is the theoretical concentration at which soil vapour and/or pore water have become fully saturated. This can indicate that NAPL is likely to be present, but for contaminants that are strongly sorbed to soils (i.e. have high  $K_{oc}$ ) and that have a low aqueous solubility and vapour pressure, exceedence of the soil saturation concentration does not necessarily imply that NAPL is present.

### 3.6 Contaminants For Which GAC Were Not Derived

As discussed in Section 3.5, GAC were not produced for the residential or allotment land-uses for the metals. GAC were not produced for any land-uses for 9 of the researched organic contaminants. The reasons for this are presented in Table 3.3 below:

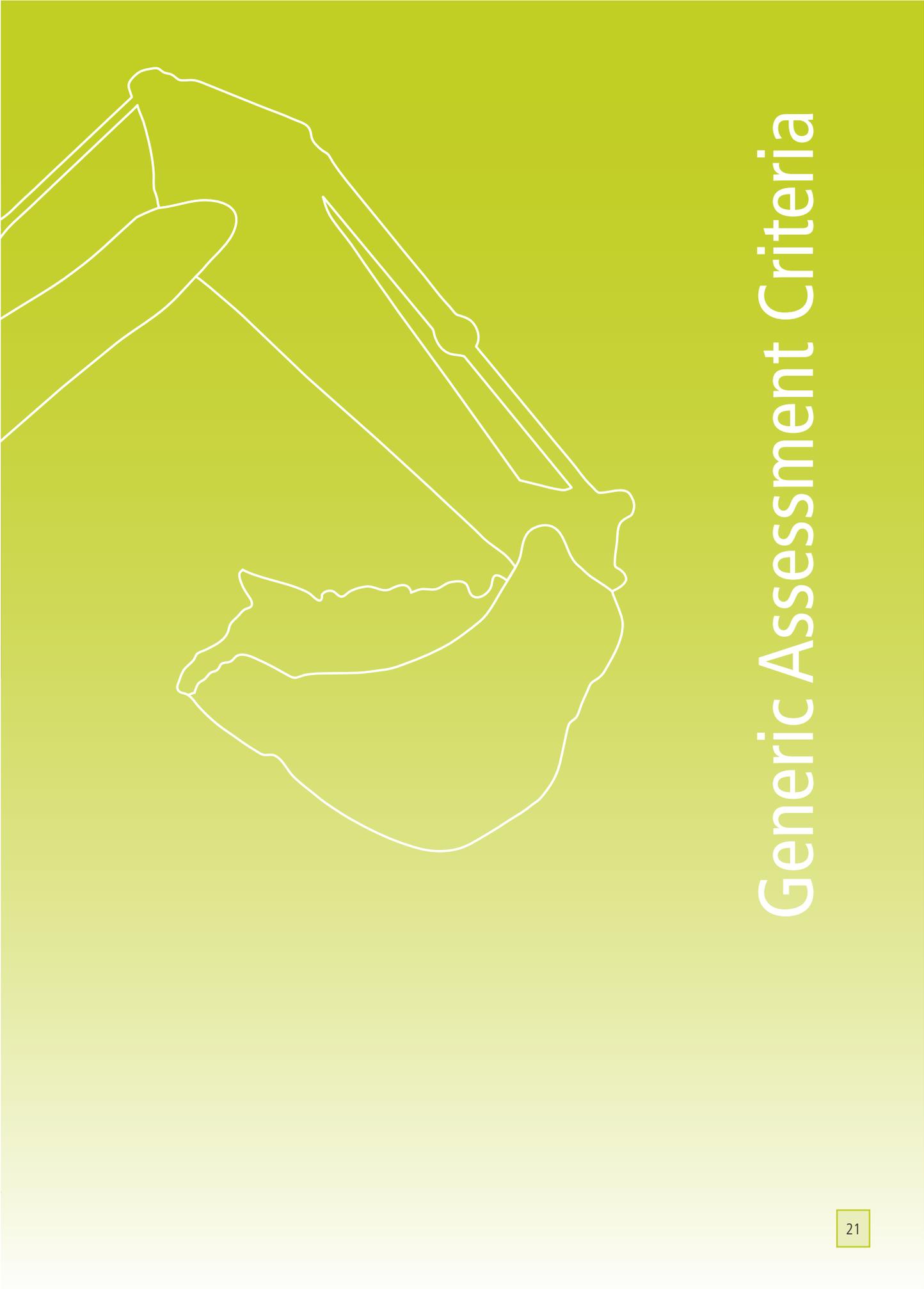
Table 3.3: Reasons for not producing GAC

Contaminant	Reason for not producing GAC
1-Methylnaphthalene	Insufficient data were available to agree a HCV for the inhalation route of exposure for these isomers. There is evidence to suggest that these substances are significantly more toxic when inhaled than when ingested. Furthermore, the CLEA model predicts inhalation to be a significant route of exposure for them. For these reasons, route-to-route extrapolation was considered inappropriate and no GAC have been derived.
2-Methylnaphthalene	
1,3,5-Trimethylbenzene	Insufficient data were available to agree HCV and thus GAC were not derived for these substances.
Carbazole	
Dimethyl phthalate	
Isopropyltoluene	
<i>n</i> butylbenzene	
<i>sec</i> butylbenzene	
<i>tert</i> butylbenzene	

### 3.7 Notes on Specific Contaminants

There are some specific issues that should be considered with the following contaminants when using the GAC:

- Methylphenols (cresols). The HCV for 2-methylphenol, 3-methylphenol and 4-methylphenol are based on the minimum risk level (MRL) set by the US Agency for Toxic Substances and Disease Registry (ATSDR) for total cresols. GAC have been derived for each individual isomer and the lowest of these chosen as the GAC for total cresols;
- Di-*n*-butyl phthalate. The  $TDI_{inhal}$  is based on localised toxicological effects in the upper respiratory tract. For this reason, the lowest of the assessment criteria derived using the oral and inhalation HCV have been used as the GAC rather than using the "combined" GAC; and
- Phthalates. The potential additivity of phthalates should be considered by assessors when using the GAC for these substances. Guidance on additivity is provided in the Environment Agency of England and Wales SR2 document.



# Generic Assessment Criteria

## 4 EIC/AGS/CL:AIRE Generic Assessment Criteria

Table 4.1a: EIC/AGS/CL:AIRE GAC for metals

Contaminant	GAC (mg.kg <sup>-1</sup> )				Soil Saturation Concentration (mg.kg <sup>-1</sup> )
	Residential with consumption of homegrown produce	Residential without consumption of homegrown produce	Allotments	Commercial	
Antimony	ND	550	ND	7500	NA
Barium	ND	1300	ND	22000	NA
Molybdenum	ND	670	ND	17000	NA

### Notes

It is strongly recommended that the accompanying EIC/AGS/CL:AIRE GAC report is read and understood if using these GAC

These GAC are not soil organic matter dependent

ND: Not derived (see Section 3.4)

NA: Not applicable

Table 4.1b: Pathway exposure contributions (%) for metals for residential landuse without consumption of homegrown produce

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral back-ground	Inhalation back-ground
Antimony	96.1	0.0	0.0	0.3	0.0	3.3	0.3
Barium	49.8	0.0	0.0	0.2	0.0	50.0	0.0
Molybdenum	49.9	0.0	0.0	0.2	0.0	49.9	0.0

Table 4.1c: Pathway exposure contributions (%) for metals for commercial landuse

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral back-ground	Inhalation back-ground
Antimony	98.2	0.0	0.0	0.6	0.0	1.0	0.2
Barium	49.7	0.0	0.0	0.3	0.0	50.0	0.0
Molybdenum	80.1	0.0	0.0	0.5	0.0	19.4	0.0

Table 4.2a: EIC/AGS/CL:AIRE GAC for organics with 1% SOM

Contaminant	GAC for 1% SOM (mg.kg <sup>-1</sup> )				Soil Saturation Concentration (mg.kg <sup>-1</sup> )
	Residential with consumption of homegrown produce	Residential without consumption of homegrown produce	Allotments	Commercial	
1,1,2 Trichloroethane	0.6	0.88	0.28	94	4030
1,1-Dichloroethane	2.4	2.5	9.2	280	1830
1,1-Dichloroethene	0.23	0.23	2.8	26	2230
1,2,4-Trimethylbenzene	0.35	0.41	0.38	42	557
1,2-Dichloropropane	0.024	0.024	0.62	3.3	1190
2,4-Dimethylphenol	19	210	3.1	16000	1380
2,4-Dinitrotoluene	1.5	170	0.22	3700	141
2,6-Dinitrotoluene	0.78	78	0.12	1900	287
2-Chloronaphthalene	3.7	3.8	40	390	114
Biphenyl	66	220	14	18000	34.4
Bis (2-ethylhexyl) phthalate	280	2700	47	85000	8.68
Bromobenzene	0.87	0.91	3.2	97	853
Bromodichloromethane	0.016	0.019	0.016	2.1	1790
Bromoform	2.8	5.2	0.95	760	2690
Butyl benzyl phthalate	1400	42000	220	940000	26.3
Chloroethane	8.3	8.4	110	960	2610
Chloromethane	0.0083	0.0085	0.066	1.0	1910
<i>Cis</i> 1,2 Dichloroethene	0.11	0.12	0.26	14	3940
Dichloromethane	0.58	2.1	0.10	270	7270
Diethyl Phthalate	120	1800	19	150000	13.7
Di- <i>n</i> -butyl phthalate	13	450	2.0	15000	4.65
Di- <i>n</i> -octyl phthalate	2300	3400	940	89000	32.6
Hexachloroethane	0.20	0.22	0.27	22	8.17
Isopropylbenzene	11	12	32	1400	390
Methyl <i>tert</i> -butyl ether	49	73	23	7900	20400
Propylbenzene	34	40	34	4100	402
Styrene	8.1	35	1.6	3300	626
Total Cresols (2-, 3- and 4-methylphenol)	80	3700	12	160000	15000
<i>Trans</i> 1,2 Dichloroethene	0.19	0.19	0.93	22	3420
Tributyl tin oxide	0.25	1.4	0.042	130	41.3

Notes

It is strongly recommended that the accompanying EIC/AGS/CL:AIRE GAC report is read and understood if using these GAC

GAC in highlighted boxes exceed soil saturation concentration. Soil concentrations above soil saturation may indicate that NAPL is present. Risks from NAPL may need to be considered separately.

Table 4.2b: Pathway exposure contributions (%) for organics for residential landuse with consumption of homegrown produce and 1% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.1	27.5	0.1	0.0	70.8	0.3	1.3
1,1-Dichloroethane	0.0	3.9	0.0	0.0	95.4	0.7	0.0
1,1-Dichloroethene	0.0	1.0	0.0	0.0	98.4	0.6	0.0
1,2,4-Trimethylbenzene	0.1	7.0	0.1	0.0	42.8	0.0	50.0
1,2-Dichloropropane	0.0	5.4	0.0	0.0	64.5	5.4	24.8
2,4-Dimethylphenol	0.7	91.0	0.4	0.0	8.0	0.0	0.0
2,4-Dinitrotoluene	0.6	99.1	0.3	0.0	0.1	0.0	0.0
2,6-Dinitrotoluene	0.6	99.0	0.3	0.0	0.1	0.0	0.0
2-Chloronaphthalene	2.0	76.9	1.0	0.0	20.0	0.0	0.1
Biphenyl	1.3	69.6	0.7	0.0	27.7	0.8	0.0
Bis (2-ethylhexyl) phthalate	4.2	57.6	2.2	0.0	0.5	35.6	0.0
Bromobenzene	0.2	23.0	0.1	0.0	76.8	0.0	0.0
Bromodichloromethane	0.0	15.2	0.0	0.0	84.7	0.0	0.0
Bromoform	0.1	30.1	0.1	0.0	36.7	33.0	0.0
Butyl benzyl phthalate	2.1	96.6	1.1	0.0	0.2	0.1	0.0
Chloroethane	0.0	1.1	0.0	0.0	98.9	0.0	0.0
Chloromethane	0.0	0.9	0.0	0.0	49.1	0.0	50.0
Cis 1,2 Dichloroethene	0.0	5.8	0.0	0.0	84.4	9.8	0.0
Dichloromethane	0.0	4.5	0.0	0.0	53.6	4.5	37.4
Diethyl Phthalate	0.4	91.5	0.2	0.0	5.5	2.3	0.0
Di- <i>n</i> -butyl phthalate	1.0	47.9	0.5	0.0	1.2	49.4	0.1
Di- <i>n</i> -octyl phthalate	33.4	25.7	17.2	0.1	0.0	23.6	0.0
Hexachloroethane	0.2	5.5	0.1	0.0	44.3	50.0	0.0
Isopropylbenzene	0.1	4.5	0.0	0.0	79.8	0.0	15.6
Methyl <i>tert</i> -butyl ether	0.1	16.6	0.0	0.0	81.2	0.0	2.1
Propylbenzene	0.1	7.5	0.1	0.0	91.8	0.0	0.5
Styrene	0.1	14.8	0.1	0.0	84.6	0.1	0.4
Total Cresols (2-, 3- and 4-methylphenol)	0.6	97.8	0.3	0.0	1.2	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	2.9	0.0	0.0	93.6	1.3	2.1
Tributyl tin oxide	0.8	48.6	0.4	0.0	0.4	49.8	0.0

Table 4.2c: Pathway exposure contributions (%) for organics for residential landuse without consumption of homegrown produce and 1% SOM

Contaminant	direct soil ingestion	sum of consumption of homegrown produce and attached soil	dermal contact (indoor and outdoor combined)	inhalation of dust (indoor and outdoor combined)	inhalation of vapour (indoor and outdoor combined)	oral background	inhalation background
1,1,2 Trichloroethane	0.1	0.0	0.1	0.0	98.4	0.2	1.3
1,1-Dichloroethane	0.0	0.0	0.0	0.0	99.3	0.7	0.0
1,1-Dichloroethene	0.0	0.0	0.0	0.0	100.0	0.0	0.0
1,2,4-Trimethylbenzene	0.2	0.0	0.1	0.0	49.8	0.0	50.0
1,2-Dichloropropane	0.0	0.0	0.0	0.0	72.3	0.0	27.6
2,4-Dimethylphenol	7.7	0.0	3.9	0.0	88.4	0.0	0.0
2,4-Dinitrotoluene	61.3	0.0	32.1	0.2	6.4	0.0	0.0
2,6-Dinitrotoluene	57.8	0.0	29.4	0.2	12.6	0.0	0.0
2-Chloronaphthalene	8.6	0.0	4.4	0.0	86.7	0.0	0.4
Biphenyl	4.3	0.0	2.2	0.0	92.7	0.8	0.0
Bis (2-ethylhexyl) phthalate	39.4	0.0	20.3	0.1	4.6	35.6	0.0
Bromobenzene	0.2	0.0	0.1	0.0	99.7	0.0	0.0
Bromodichloromethane	0.1	0.0	0.0	0.0	99.9	0.0	0.0
Bromoform	0.2	0.0	0.1	0.0	66.7	33.0	0.0
Butyl benzyl phthalate	62.9	0.0	32.3	0.2	4.5	0.1	0.0
Chloroethane	0.0	0.0	0.0	0.0	100.0	0.0	0.0
Chloromethane	0.0	0.0	0.0	0.0	50.0	0.0	50.0
<i>Cis 1,2 Dichloroethene</i>	0.0	0.0	0.0	0.0	90.2	9.8	0.0
Dichloromethane	0.0	0.0	0.0	0.0	84.1	0.0	15.8
Diethyl Phthalate	6.8	0.0	3.5	0.0	87.3	2.3	0.0
Di- <i>n</i> -butyl phthalate	23.2	0.0	11.9	0.1	29.7	35.1	0.1
Di- <i>n</i> -octyl phthalate	50.3	0.0	25.9	0.2	0.0	23.6	0.0
Hexachloroethane	0.2	0.0	0.1	0.0	49.8	50.0	0.0
Isopropylbenzene	0.1	0.0	0.0	0.0	84.3	0.0	15.6
Methyl <i>tert</i> -butyl ether	0.1	0.0	0.0	0.0	98.2	0.0	1.7
Propylbenzene	0.1	0.0	0.1	0.0	99.3	0.0	0.5
Styrene	0.1	0.0	0.1	0.0	99.7	0.0	0.1
Total Cresols (2-, 3- and 4-methylphenol)	28.1	0.0	14.4	0.1	57.4	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	0.0	0.0	0.0	97.8	0.0	2.1
Tributyl tin oxide	28.4	0.0	14.6	0.1	14.0	43.0	0.0

Table 4.2d: Pathway exposure contributions (%) for organics for allotments and 1% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.0	99.6	0.0	0.0	0.0	0.3	0.0
1,1-Dichloroethane	0.0	99.3	0.0	0.0	0.0	0.7	0.0
1,1-Dichloroethene	0.0	99.1	0.0	0.0	0.1	0.7	0.1
1,2,4-Trimethylbenzene	0.0	49.9	0.0	0.0	0.0	0.0	50.0
1,2-Dichloropropane	0.0	84.7	0.0	0.0	0.0	15.3	0.0
2,4-Dimethylphenol	0.0	100.0	0.0	0.0	0.0	0.0	0.0
2,4-Dinitrotoluene	0.0	100.0	0.0	0.0	0.0	0.0	0.0
2,6-Dinitrotoluene	0.0	100.0	0.0	0.0	0.0	0.0	0.0
2-Chloronaphthalene	0.1	99.8	0.1	0.0	0.0	0.0	0.0
Biphenyl	0.1	99.1	0.0	0.0	0.0	0.8	0.0
Bis (2-ethylhexyl) phthalate	0.2	64.1	0.1	0.0	0.0	35.6	0.0
Bromobenzene	0.0	99.9	0.0	0.0	0.0	0.0	0.0
Bromodichloromethane	0.0	100.0	0.0	0.0	0.0	0.0	0.0
Bromoform	0.0	67.0	0.0	0.0	0.0	33.0	0.0
Butyl benzyl phthalate	0.1	99.8	0.0	0.0	0.0	0.1	0.0
Chloroethane	0.0	99.9	0.0	0.0	0.1	0.0	0.0
Chloromethane	0.0	50.0	0.0	0.0	0.0	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.0	90.2	0.0	0.0	0.0	9.8	0.0
Dichloromethane	0.0	50.0	0.0	0.0	0.0	50.0	0.0
Diethyl Phthalate	0.0	97.6	0.0	0.0	0.0	2.3	0.0
Di- <i>n</i> -butyl phthalate	0.0	49.9	0.0	0.0	0.0	50.0	0.0
Di- <i>n</i> -octyl phthalate	3.7	70.8	1.9	0.0	0.0	23.6	0.0
Hexachloroethane	0.1	49.9	0.0	0.0	0.0	50.0	0.0
Isopropylbenzene	0.1	99.8	0.0	0.0	0.1	0.0	0.1
Methyl <i>tert</i> -butyl ether	0.0	99.9	0.0	0.0	0.0	0.0	0.0
Propylbenzene	0.1	99.8	0.0	0.0	0.1	0.0	0.1
Styrene	0.0	99.4	0.0	0.0	0.0	0.5	0.0
Total Cresols (2-, 3- and 4-methylphenol)	0.0	99.9	0.0	0.0	0.0	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	98.6	0.0	0.0	0.0	1.3	0.0
Tributyl tin oxide	0.0	50.0	0.0	0.0	0.0	50.0	0.0

Table 4.2e: Pathway exposure contributions (%) for organics for commercial landuse and 1% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.9	0.0	0.2	0.0	98.6	0.1	0.3
1,1-Dichloroethane	0.1	0.0	0.0	0.0	99.8	0.2	0.0
1,1-Dichloroethene	0.0	0.0	0.0	0.0	99.9	0.0	0.0
1,2,4-Trimethylbenzene	0.9	0.0	0.2	0.0	48.9	0.0	50.0
1,2-Dichloropropane	0.1	0.0	0.0	0.0	93.2	0.2	6.5
2,4-Dimethylphenol	36.6	0.0	6.1	0.2	57.1	0.0	0.0
2,4-Dinitrotoluene	83.9	0.0	14.1	0.5	1.4	0.0	0.0
2,6-Dinitrotoluene	83.6	0.0	13.7	0.5	2.3	0.0	0.0
2-Chloronaphthalene	36.0	0.0	5.9	0.2	57.8	0.0	0.1
Biphenyl	21.7	0.0	3.6	0.1	74.4	0.2	0.0
Bis (2-ethylhexyl) phthalate	76.7	0.0	12.7	0.5	1.1	9.0	0.0
Bromobenzene	1.3	0.0	0.2	0.0	98.5	0.0	0.0
Bromodichloromethane	0.3	0.0	0.1	0.0	99.6	0.0	0.0
Bromoform	1.7	0.0	0.3	0.0	90.0	8.0	0.0
Butyl benzyl phthalate	84.7	0.0	14.0	0.5	0.7	0.0	0.0
Chloroethane	0.0	0.0	0.0	0.0	100.0	0.0	0.0
Chloromethane	0.0	0.0	0.0	0.0	50.0	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.1	0.0	0.0	0.0	97.5	2.4	0.0
Dichloromethane	0.1	0.0	0.0	0.0	96.0	0.1	3.8
Diethyl Phthalate	33.7	0.0	5.6	0.2	60.0	0.6	0.0
Di- <i>n</i> -butyl phthalate	61.1	0.0	10.1	0.4	11.7	16.7	0.0
Di- <i>n</i> -octyl phthalate	80.2	0.0	13.3	0.5	0.0	6.0	0.0
Hexachloroethane	1.0	0.0	0.2	0.0	48.8	50.0	0.0
Isopropylbenzene	0.5	0.0	0.1	0.0	95.7	0.0	3.7
Methyl <i>tert</i> -butyl ether	0.5	0.0	0.1	0.0	99.0	0.0	0.4
Propylbenzene	0.9	0.0	0.1	0.0	98.9	0.0	0.1
Styrene	0.7	0.0	0.1	0.0	99.1	0.0	0.0
Total Cresols (2-, 3- and 4-methylphenol)	73.4	0.0	12.1	0.5	14.0	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.1	0.0	0.0	0.0	99.4	0.1	0.5
Tributyl tin oxide	41.8	0.0	6.9	0.3	2.4	48.7	0.0

Table 4.3a: EIC/AGS/CL:AIRE GAC for organics with 2.5% SOM

Contaminant	GAC for 2.5% SOM (mg.kg <sup>-1</sup> )				Soil Saturation Concentration (mg.kg <sup>-1</sup> )
	Residential with consumption of homegrown produce	Residential without consumption of homegrown produce	Allotments	Commercial	
1,1,2 Trichloroethane	1.2	1.8	0.61	190	8210
1,1-Dichloroethane	3.9	4.1	17	450	2960
1,1-Dichloroethene	0.40	0.41	5.6	46	3940
1,2,4-Trimethylbenzene	0.85	0.99	0.93	99	1360
1,2-Dichloropropane	0.042	0.042	1.2	5.9	2110
2,4-Dimethylphenol	43	410	7.2	24000	3140
2,4-Dinitrotoluene	3.2	170	0.49	3700	299
2,6-Dinitrotoluene	1.7	84	0.27	1900	622
2-Chloronaphthalene	9.2	9.3	98	960	280
Biphenyl	160	500	35	33000	84.3
Bis (2-ethylhexyl) phthalate	610	2800	120	86000	21.6
Bromobenzene	2.0	2.1	7.6	220	1970
Bromodichloromethane	0.030	0.034	0.032	3.7	3220
Bromoform	5.9	11	2.1	1500	5480
Butyl benzyl phthalate	3300	44000	550	940000	64.7
Chloroethane	11	11	200	1300	3540
Chloromethane	0.0098	0.0099	0.13	1.2	2240
<i>Cis</i> 1,2 Dichloroethene	0.19	0.20	0.50	24	6610
Dichloromethane	0.98	2.8	0.19	360	9680
Diethyl Phthalate	260	3500	41	220000	29.1
Di- <i>n</i> -butyl phthalate	31	450	5.0	15000	11.4
Di- <i>n</i> -octyl phthalate	2800	3400	2100	89000	81.5
Hexachloroethane	0.48	0.54	0.67	53	20.1
Isopropylbenzene	27	28	79	3300	950
Methyl <i>tert</i> -butyl ether	84	120	44	13000	33100
Propylbenzene	82	97	83	9700	981
Styrene	19	78	3.7	6500	1440
Total Cresols (2-, 3- and 4-methylphenol)	180	5400	27	180000	32500
<i>Trans</i> 1,2 Dichloroethene	0.34	0.35	1.9	40	6170
Tributyl tin oxide	0.59	3.1	0.10	180	101

#### Notes

It is strongly recommended that the accompanying EIC/AGS/CL:AIRE GAC report is read and understood if using these GAC.

GAC in highlighted boxes exceed soil saturation concentration. Soil concentrations above soil saturation may indicate that NAPL is present. Risks from NAPL may need to be considered separately.

Table 4.3b: Pathway exposure contributions (%) for organics for residential landuse with consumption of homegrown produce and 2.5% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.2	26.2	0.1	0.0	71.9	0.3	1.3
1,1-Dichloroethane	0.0	3.4	0.0	0.0	95.9	0.7	0.0
1,1-Dichloroethene	0.0	0.9	0.0	0.0	98.5	0.6	0.0
1,2,4-Trimethylbenzene	0.3	6.9	0.2	0.0	42.6	0.0	50.0
1,2-Dichloropropane	0.0	4.8	0.0	0.0	65.2	4.9	25.0
2,4-Dimethylphenol	1.6	89.5	0.8	0.0	8.1	0.0	0.0
2,4-Dinitrotoluene	1.2	98.1	0.6	0.0	0.1	0.0	0.0
2,6-Dinitrotoluene	1.3	97.9	0.7	0.0	0.1	0.0	0.0
2-Chloronaphthalene	4.7	73.6	2.4	0.0	19.2	0.0	0.1
Biphenyl	3.1	67.5	1.6	0.0	27.1	0.8	0.0
Bis (2-ethylhexyl) phthalate	9.1	50.2	4.7	0.0	0.4	35.6	0.0
Bromobenzene	0.4	22.4	0.2	0.0	77.1	0.0	0.0
Bromodichloromethane	0.1	13.9	0.0	0.0	86.0	0.0	0.0
Bromoform	0.2	29.0	0.1	0.0	37.6	33.0	0.0
Butyl benzyl phthalate	5.0	92.2	2.6	0.0	0.1	0.1	0.0
Chloroethane	0.0	0.8	0.0	0.0	99.2	0.0	0.0
Chloromethane	0.0	0.6	0.0	0.0	49.4	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.0	5.1	0.0	0.0	85.0	9.8	0.0
Dichloromethane	0.0	3.7	0.0	0.0	59.9	3.7	32.8
Diethyl Phthalate	1.0	90.5	0.5	0.0	5.7	2.3	0.0
Di- <i>n</i> -butyl phthalate	2.3	46.0	1.2	0.0	1.2	49.4	0.1
Di- <i>n</i> -octyl phthalate	41.7	13.1	21.4	0.1	0.0	23.6	0.0
Hexachloroethane	0.4	5.4	0.2	0.0	44.1	50.0	0.0
Isopropylbenzene	0.2	4.5	0.1	0.0	79.7	0.0	15.6
Methyl <i>tert</i> -butyl ether	0.1	14.4	0.1	0.0	83.5	0.0	2.0
Propylbenzene	0.3	7.4	0.2	0.0	91.6	0.0	0.5
Styrene	0.2	14.4	0.1	0.0	84.8	0.1	0.4
Total Cresols (2-, 3- and 4-methylphenol)	1.3	96.7	0.7	0.0	1.3	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	2.7	0.0	0.0	93.9	1.3	2.1
Tributyl tin oxide	1.9	46.9	1.0	0.0	0.4	49.8	0.0

Table 4.3c: Pathway exposure contributions (%) for organics for residential landuse without consumption of homegrown produce and 2.5% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.3	0.0	0.1	0.0	98.1	0.3	1.3
1,1-Dichloroethane	0.0	0.0	0.0	0.0	99.3	0.7	0.0
1,1-Dichloroethene	0.0	0.0	0.0	0.0	99.9	0.0	0.0
1,2,4-Trimethylbenzene	0.4	0.0	0.2	0.0	49.4	0.0	50.0
1,2-Dichloropropane	0.0	0.0	0.0	0.0	72.3	0.0	27.6
2,4-Dimethylphenol	15.2	0.0	7.8	0.1	77.0	0.0	0.0
2,4-Dinitrotoluene	63.4	0.0	33.3	0.2	3.1	0.0	0.0
2,6-Dinitrotoluene	62.0	0.0	31.6	0.2	6.2	0.0	0.0
2-Chloronaphthalene	17.7	0.0	9.1	0.1	72.8	0.0	0.3
Biphenyl	9.7	0.0	5.0	0.0	84.6	0.8	0.0
Bis (2-ethylhexyl) phthalate	41.2	0.0	21.2	0.1	1.9	35.6	0.0
Bromobenzene	0.5	0.0	0.2	0.0	99.3	0.0	0.0
Bromodichloromethane	0.1	0.0	0.0	0.0	99.9	0.0	0.0
Bromoform	0.4	0.0	0.2	0.0	66.4	33.0	0.0
Butyl benzyl phthalate	64.6	0.0	33.2	0.2	1.9	0.1	0.0
Chloroethane	0.0	0.0	0.0	0.0	100.0	0.0	0.0
Chloromethane	0.0	0.0	0.0	0.0	50.0	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.0	0.0	0.0	0.0	90.2	9.8	0.0
Dichloromethane	0.0	0.0	0.0	0.0	84.1	0.0	15.9
Diethyl Phthalate	13.0	0.0	6.7	0.0	78.0	2.3	0.0
Di- <i>n</i> -butyl phthalate	28.2	0.0	14.5	0.1	14.6	42.6	0.1
Di- <i>n</i> -octyl phthalate	50.3	0.0	25.9	0.2	0.0	23.6	0.0
Hexachloroethane	0.4	0.0	0.2	0.0	49.4	50.0	0.0
Isopropylbenzene	0.2	0.0	0.1	0.0	84.1	0.0	15.6
Methyl <i>tert</i> -butyl ether	0.1	0.0	0.1	0.0	98.1	0.0	1.7
Propylbenzene	0.3	0.0	0.2	0.0	99.1	0.0	0.5
Styrene	0.3	0.0	0.1	0.0	99.4	0.0	0.1
Total Cresols (2-, 3- and 4-methylphenol)	40.5	0.0	20.8	0.1	38.5	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	0.0	0.0	0.0	97.8	0.0	2.1
Tributyl tin oxide	30.9	0.0	15.9	0.1	6.2	46.8	0.0

Table 4.3d: Pathway exposure contributions (%) for organics for allotments and 2.5% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.0	99.6	0.0	0.0	0.0	0.3	0.0
1,1-Dichloroethane	0.0	99.2	0.0	0.0	0.1	0.7	0.0
1,1-Dichloroethene	0.0	99.1	0.0	0.0	0.1	0.7	0.1
1,2,4-Trimethylbenzene	0.1	49.8	0.1	0.0	0.0	0.0	50.0
1,2-Dichloropropane	0.0	84.6	0.0	0.0	0.0	15.3	0.0
2,4-Dimethylphenol	0.1	99.9	0.0	0.0	0.0	0.0	0.0
2,4-Dinitrotoluene	0.1	99.9	0.0	0.0	0.0	0.0	0.0
2,6-Dinitrotoluene	0.1	99.9	0.0	0.0	0.0	0.0	0.0
2-Chloronaphthalene	0.3	99.6	0.1	0.0	0.0	0.0	0.0
Biphenyl	0.2	99.0	0.1	0.0	0.0	0.8	0.0
Bis (2-ethylhexyl) phthalate	0.5	63.7	0.2	0.0	0.0	35.6	0.0
Bromobenzene	0.1	99.9	0.0	0.0	0.0	0.0	0.0
Bromodichloromethane	0.0	99.9	0.0	0.0	0.0	0.0	0.0
Bromoform	0.0	66.9	0.0	0.0	0.0	33.0	0.0
Butyl benzyl phthalate	0.2	99.6	0.1	0.0	0.0	0.1	0.0
Chloroethane	0.0	99.9	0.0	0.0	0.1	0.0	0.0
Chloromethane	0.0	50.0	0.0	0.0	0.0	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.0	90.1	0.0	0.0	0.0	9.8	0.0
Dichloromethane	0.0	50.0	0.0	0.0	0.0	50.0	0.0
Diethyl Phthalate	0.0	97.6	0.0	0.0	0.0	2.3	0.0
Di- <i>n</i> -butyl phthalate	0.1	49.9	0.1	0.0	0.0	50.0	0.0
Di- <i>n</i> -octyl phthalate	8.3	64.0	4.1	0.0	0.0	23.6	0.0
Hexachloroethane	0.1	49.8	0.1	0.0	0.1	50.0	0.0
Isopropylbenzene	0.2	99.5	0.1	0.0	0.1	0.0	0.1
Methyl <i>tert</i> -butyl ether	0.0	99.9	0.0	0.0	0.0	0.0	0.0
Propylbenzene	0.2	99.6	0.1	0.0	0.1	0.0	0.1
Styrene	0.1	99.4	0.0	0.0	0.0	0.5	0.0
Total Cresols (2-, 3- and 4-methylphenol)	0.1	99.9	0.0	0.0	0.0	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	98.5	0.0	0.0	0.1	1.3	0.1
Tributyl tin oxide	0.1	49.9	0.0	0.0	0.0	50.0	0.0

Table 4.3e: Pathway exposure contributions (%) for organics for commercial landuse and 2.5% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	1.8	0.0	0.3	0.0	97.6	0.1	0.3
1,1-Dichloroethane	0.1	0.0	0.0	0.0	99.7	0.2	0.0
1,1-Dichloroethene	0.0	0.0	0.0	0.0	99.9	0.0	0.0
1,2,4-Trimethylbenzene	2.2	0.0	0.4	0.0	47.4	0.0	50.0
1,2-Dichloropropane	0.2	0.0	0.0	0.0	93.0	0.3	6.5
2,4-Dimethylphenol	53.8	0.0	8.9	0.3	37.0	0.0	0.0
2,4-Dinitrotoluene	84.4	0.0	14.2	0.5	0.9	0.0	0.0
2,6-Dinitrotoluene	84.4	0.0	13.8	0.5	1.2	0.0	0.0
2-Chloronaphthalene	54.8	0.0	9.1	0.4	35.8	0.0	0.0
Biphenyl	38.8	0.0	6.4	0.3	54.4	0.2	0.0
Bis (2-ethylhexyl) phthalate	77.3	0.0	12.8	0.5	0.5	9.0	0.0
Bromobenzene	2.9	0.0	0.5	0.0	96.7	0.0	0.0
Bromodichloromethane	0.6	0.0	0.1	0.0	99.3	0.0	0.0
Bromoform	3.4	0.0	0.6	0.0	88.0	8.0	0.0
Butyl benzyl phthalate	85.0	0.0	14.0	0.5	0.4	0.0	0.0
Chloroethane	0.0	0.0	0.0	0.0	100.0	0.0	0.0
Chloromethane	0.0	0.0	0.0	0.0	50.0	0.0	50.0
Cis 1,2 Dichloroethene	0.2	0.0	0.0	0.0	97.4	2.4	0.0
Dichloromethane	0.1	0.0	0.0	0.0	95.9	0.1	3.8
Diethyl Phthalate	49.4	0.0	8.2	0.3	41.5	0.6	0.0
Di- <i>n</i> -butyl phthalate	65.6	0.0	10.8	0.4	5.1	17.9	0.0
Di- <i>n</i> -octyl phthalate	80.2	0.0	13.3	0.5	0.0	6.0	0.0
Hexachloroethane	2.4	0.0	0.4	0.0	47.2	50.0	0.0
Isopropylbenzene	1.3	0.0	0.2	0.0	94.8	0.0	3.7
Methyl <i>tert</i> -butyl ether	0.8	0.0	0.1	0.0	98.7	0.0	0.4
Propylbenzene	2.0	0.0	0.3	0.0	97.5	0.0	0.1
Styrene	1.7	0.0	0.3	0.0	98.0	0.0	0.0
Total Cresols (2-, 3- and 4-methylphenol)	79.2	0.0	13.1	0.5	7.2	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.1	0.0	0.0	0.0	99.3	0.1	0.5
Tributyl tin oxide	42.4	0.0	7.0	0.3	1.0	49.4	0.0

Table 4.4a: EIC/AGS/CL:AIRE GAC for organics with 6% SOM

Contaminant	GAC for 6% SOM (mg.kg <sup>-1</sup> )				Soil Saturation Concentration (mg.kg <sup>-1</sup> )
	Residential with consumption of homegrown produce	Residential without consumption of homegrown produce	Allotments	Commercial	
1,1,2 Trichloroethane	2.7	3.9	1.4	400	18000
1,1-Dichloroethane	7.4	7.7	35	850	5600
1,1-Dichloroethene	0.82	0.82	12	92	7940
1,2,4-Trimethylbenzene	2.0	2.3	2.2	220	3250
1,2-Dichloropropane	0.084	0.085	2.6	12	4240
2,4-Dimethylphenol	97	730	17	30000	7240
2,4-Dinitrotoluene	7.2	170	1.1	3800	669
2,6-Dinitrotoluene	3.9	87	0.61	1900	1400
2-Chloronaphthalene	22	22	230	2200	669
Biphenyl	360	980	83	48000	201
Bis (2-ethylhexyl) phthalate	1100	2800	280	86000	51.7
Bromobenzene	4.7	4.9	18	520	4580
Bromodichloromethane	0.061	0.070	0.068	7.6	6570
Bromoform	13	23	4.6	3100	12000
Butyl benzyl phthalate	7200	44000	1300	950000	154
Chloroethane	18	18	380	2100	5710
Chloromethane	0.013	0.013	0.23	1.6	2990
Cis 1,2 Dichloroethene	0.37	0.39	1.0	47	12900
Dichloromethane	1.7	4.5	0.34	560	15300
Diethyl Phthalate	570	6300	94	290000	65
Di- <i>n</i> -butyl phthalate	67	450	12	15000	27.3
Di- <i>n</i> -octyl phthalate	3100	3400	3900	89000	196
Hexachloroethane	1.1	1.3	1.6	120	48.1
Isopropylbenzene	64	67	190	7700	2250
Methyl <i>tert</i> -butyl ether	160	220	90	24000	62700
Propylbenzene	190	230	200	21000	2330
Styrene	43	170	8.7	11000	3350
Total Cresols (2-, 3- and 4-methylphenol)	400	6900	63	180000	73300
<i>Trans</i> 1,2 Dichloroethene	0.70	0.71	4.0	81	12600
Tributyl tin oxide	1.3	5.7	0.24	200	241

#### Notes

It is strongly recommended that the accompanying EIC/AGS/CL:AIRE GAC report is read and understood if using these GAC.

GAC in highlighted boxes exceed soil saturation concentration. Soil concentrations above soil saturation may indicate that NAPL is present. Risks from NAPL may need to be considered separately.

Table 4.4b: Pathway exposure contributions (%) for organics for residential landuse with consumption of homegrown produce and 6% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.4	25.7	0.2	0.0	72.1	0.3	1.3
1,1-Dichloroethane	0.0	3.1	0.0	0.0	96.1	0.7	0.0
1,1-Dichloroethene	0.0	0.8	0.0	0.0	98.5	0.6	0.0
1,2,4-Trimethylbenzene	0.8	6.8	0.4	0.0	42.1	0.0	50.0
1,2-Dichloropropane	0.1	4.6	0.0	0.0	65.5	4.7	25.1
2,4-Dimethylphenol	3.6	86.7	1.8	0.0	7.9	0.0	0.0
2,4-Dinitrotoluene	2.7	95.9	1.4	0.0	0.1	0.0	0.0
2,6-Dinitrotoluene	2.9	95.5	1.5	0.0	0.1	0.0	0.0
2-Chloronaphthalene	10.2	67.0	5.2	0.0	17.5	0.0	0.1
Biphenyl	6.9	63.3	3.6	0.0	25.4	0.8	0.0
Bis (2-ethylhexyl) phthalate	16.8	38.7	8.6	0.1	0.3	35.6	0.0
Bromobenzene	0.8	22.1	0.4	0.0	76.7	0.0	0.0
Bromodichloromethane	0.2	13.4	0.1	0.0	86.4	0.0	0.0
Bromoform	0.5	28.5	0.3	0.0	37.8	33.0	0.0
Butyl benzyl phthalate	10.8	83.5	5.5	0.0	0.1	0.1	0.0
Chloroethane	0.0	0.7	0.0	0.0	99.3	0.0	0.0
Chloromethane	0.0	0.4	0.0	0.0	49.6	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.1	4.9	0.0	0.0	85.3	9.8	0.0
Dichloromethane	0.0	3.3	0.0	0.0	62.6	3.3	30.7
Diethyl Phthalate	2.1	88.8	1.1	0.0	5.7	2.3	0.0
Di- <i>n</i> -butyl phthalate	4.9	42.0	2.5	0.0	1.1	49.4	0.1
Di- <i>n</i> -octyl phthalate	46.2	6.4	23.7	0.2	0.0	23.6	0.0
Hexachloroethane	0.8	5.3	0.4	0.0	43.4	50.0	0.0
Isopropylbenzene	0.4	4.4	0.2	0.0	79.4	0.0	15.6
Methyl <i>tert</i> -butyl ether	0.2	13.4	0.1	0.0	84.3	0.0	2.0
Propylbenzene	0.7	7.3	0.4	0.0	91.1	0.0	0.5
Styrene	0.5	14.2	0.3	0.0	84.5	0.1	0.4
Total Cresols (2-, 3- and 4-methylphenol)	2.9	94.3	1.5	0.0	1.2	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	2.5	0.0	0.0	94.0	1.3	2.1
Tributyl tin oxide	4.2	43.4	2.2	0.0	0.4	49.8	0.0

Table 4.4c: Pathway exposure contributions (%) for organics for residential landuse without consumption of homegrown produce and 6% SOM

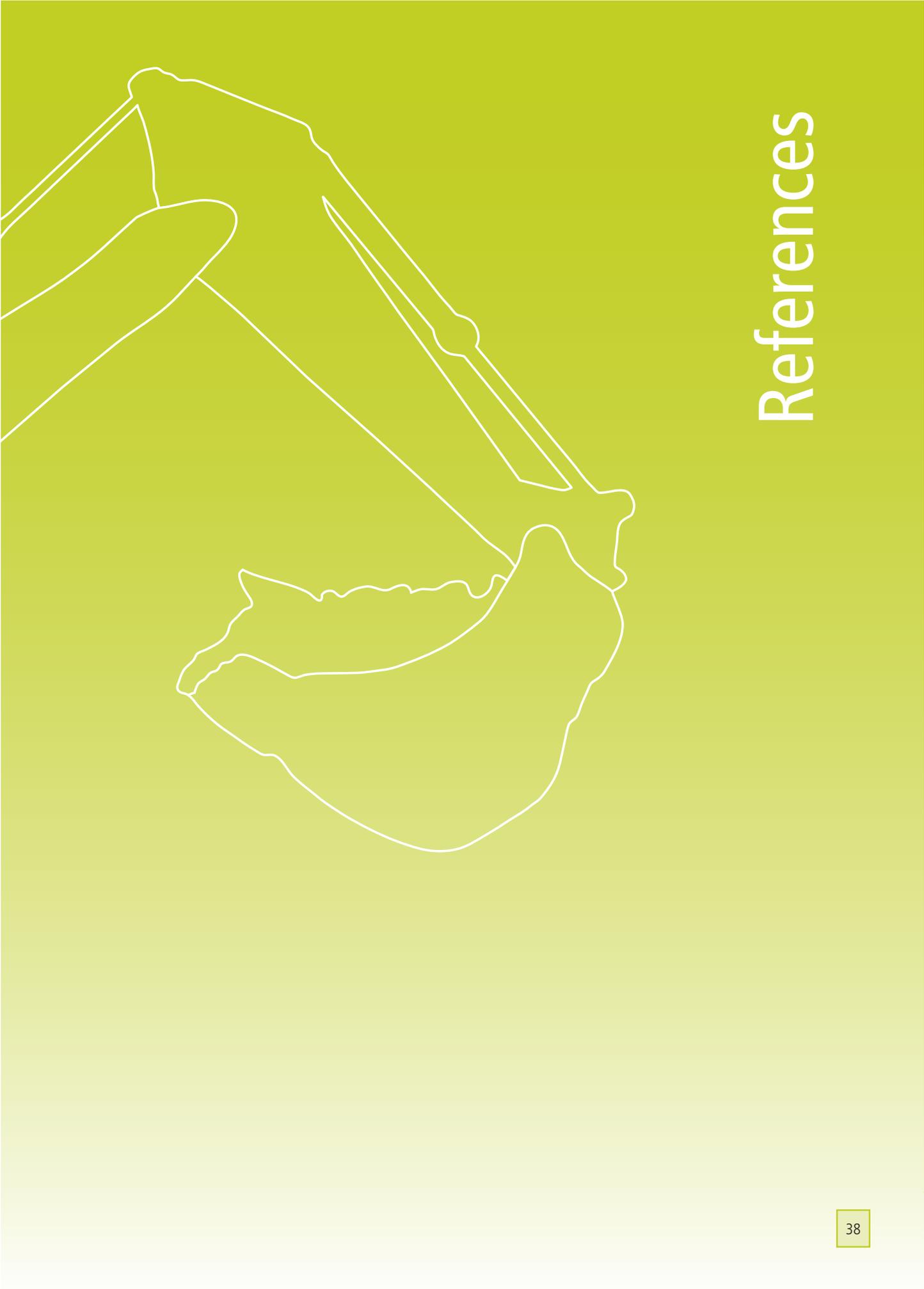
Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.6	0.0	0.3	0.0	97.6	0.3	1.3
1,1-Dichloroethane	0.0	0.0	0.0	0.0	99.3	0.7	0.0
1,1-Dichloroethene	0.0	0.0	0.0	0.0	99.9	0.0	0.0
1,2,4-Trimethylbenzene	0.9	0.0	0.4	0.0	48.7	0.0	50.0
1,2-Dichloropropane	0.1	0.0	0.0	0.0	72.2	0.1	27.6
2,4-Dimethylphenol	26.9	0.0	13.8	0.1	59.2	0.0	0.0
2,4-Dinitrotoluene	64.5	0.0	33.8	0.2	1.4	0.0	0.0
2,6-Dinitrotoluene	64.3	0.0	32.7	0.2	2.9	0.0	0.0
2-Chloronaphthalene	30.8	0.0	15.8	0.1	53.0	0.0	0.2
Biphenyl	19.2	0.0	9.8	0.1	70.2	0.8	0.0
Bis (2-ethylhexyl) phthalate	41.9	0.0	21.5	0.1	0.8	35.6	0.0
Bromobenzene	1.0	0.0	0.5	0.0	98.4	0.0	0.0
Bromodichloromethane	0.2	0.0	0.1	0.0	99.7	0.0	0.0
Bromoform	0.8	0.0	0.4	0.0	65.7	33.0	0.0
Butyl benzyl phthalate	65.3	0.0	33.6	0.2	0.8	0.1	0.0
Chloroethane	0.0	0.0	0.0	0.0	100.0	0.0	0.0
Chloromethane	0.0	0.0	0.0	0.0	50.0	0.0	50.0
Cis 1,2 Dichloroethene	0.1	0.0	0.0	0.0	90.1	9.8	0.0
Dichloromethane	0.0	0.0	0.0	0.0	84.0	0.0	15.9
Diethyl Phthalate	23.2	0.0	11.9	0.1	62.5	2.3	0.0
Di- <i>n</i> -butyl phthalate	30.8	0.0	15.8	0.1	6.7	46.6	0.1
Di- <i>n</i> -octyl phthalate	50.3	0.0	25.9	0.2	0.0	23.6	0.0
Hexachloroethane	0.9	0.0	0.5	0.0	48.6	50.0	0.0
Isopropylbenzene	0.4	0.0	0.2	0.0	83.8	0.0	15.6
Methyl <i>tert</i> -butyl ether	0.2	0.0	0.1	0.0	98.0	0.0	1.7
Propylbenzene	0.8	0.0	0.4	0.0	98.4	0.0	0.5
Styrene	0.6	0.0	0.3	0.0	98.9	0.0	0.1
Total Cresols (2-, 3- and 4-methylphenol)	51.5	0.0	26.5	0.2	21.8	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.0	0.0	0.0	0.0	97.8	0.1	2.1
Tributyl tin oxide	32.1	0.0	16.5	0.1	2.7	48.6	0.0

Table 4.4d: Pathway exposure contributions (%) for organics for allotments and 6% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	0.1	99.5	0.0	0.0	0.0	0.3	0.0
1,1-Dichloroethane	0.0	99.2	0.0	0.0	0.1	0.7	0.0
1,1-Dichloroethene	0.1	99.0	0.0	0.0	0.2	0.7	0.1
1,2,4-Trimethylbenzene	0.2	49.6	0.1	0.0	0.1	0.0	50.0
1,2-Dichloropropane	0.0	84.5	0.0	0.0	0.0	15.3	0.0
2,4-Dimethylphenol	0.2	99.7	0.1	0.0	0.0	0.0	0.0
2,4-Dinitrotoluene	0.1	99.8	0.1	0.0	0.0	0.0	0.0
2,6-Dinitrotoluene	0.1	99.8	0.1	0.0	0.0	0.0	0.0
2-Chloronaphthalene	0.6	99.1	0.3	0.0	0.0	0.0	0.0
Biphenyl	0.4	98.6	0.2	0.0	0.0	0.8	0.0
Bis (2-ethylhexyl) phthalate	1.1	62.8	0.6	0.0	0.0	35.6	0.0
Bromobenzene	0.2	99.7	0.1	0.0	0.1	0.0	0.0
Bromodichloromethane	0.1	99.9	0.0	0.0	0.0	0.0	0.0
Bromoform	0.1	66.9	0.0	0.0	0.0	33.0	0.0
Butyl benzyl phthalate	0.5	99.1	0.3	0.0	0.0	0.1	0.0
Chloroethane	0.0	99.8	0.0	0.0	0.1	0.0	0.0
Chloromethane	0.0	49.9	0.0	0.0	0.1	0.0	50.0
Cis 1,2 Dichloroethene	0.0	90.1	0.0	0.0	0.1	9.8	0.0
Dichloromethane	0.0	50.0	0.0	0.0	0.0	50.0	0.0
Diethyl Phthalate	0.1	97.5	0.1	0.0	0.0	2.3	0.0
Di- <i>n</i> -butyl phthalate	0.2	49.6	0.1	0.0	0.0	50.0	0.0
Di- <i>n</i> -octyl phthalate	15.6	53.0	7.8	0.0	0.0	23.6	0.0
Hexachloroethane	0.3	49.5	0.2	0.0	0.1	50.0	0.0
Isopropylbenzene	0.4	99.1	0.2	0.0	0.2	0.0	0.2
Methyl <i>tert</i> -butyl ether	0.1	99.8	0.0	0.0	0.0	0.0	0.0
Propylbenzene	0.4	99.1	0.2	0.0	0.1	0.0	0.2
Styrene	0.2	99.2	0.1	0.0	0.1	0.5	0.1
Total Cresols (2-, 3- and 4-methylphenol)	0.1	99.8	0.1	0.0	0.0	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.1	98.4	0.0	0.0	0.1	1.3	0.1
Tributyl tin oxide	0.2	49.7	0.1	0	0	50	0

Table 4.4e: Pathway exposure contributions (%) for organics for commercial landuse and 6% SOM

Contaminant	Direct soil ingestion	Sum of consumption of homegrown produce and attached soil	Dermal contact (indoor and outdoor combined)	Inhalation of dust (indoor and outdoor combined)	Inhalation of vapour (indoor and outdoor combined)	Oral background	Inhalation background
1,1,2 Trichloroethane	3.8	0.0	0.6	0.0	95.2	0.1	0.3
1,1-Dichloroethane	0.2	0.0	0.0	0.0	99.6	0.2	0.0
1,1-Dichloroethene	0.1	0.0	0.0	0.0	99.8	0.1	0.0
1,2,4-Trimethylbenzene	4.9	0.0	0.8	0.0	44.2	0.0	50.0
1,2-Dichloropropane	0.5	0.0	0.1	0.0	92.5	0.5	6.5
2,4-Dimethylphenol	68.0	0.0	11.2	0.4	20.4	0.0	0.0
2,4-Dinitrotoluene	84.7	0.0	14.3	0.5	0.5	0.0	0.0
2,6-Dinitrotoluene	84.9	0.0	13.9	0.5	0.7	0.0	0.0
2-Chloronaphthalene	69.1	0.0	11.4	0.4	19.0	0.0	0.0
Biphenyl	56.7	0.0	9.4	0.4	33.4	0.2	0.0
Bis (2-ethylhexyl) phthalate	77.5	0.0	12.8	0.5	0.2	9.0	0.0
Bromobenzene	6.3	0.0	1.1	0.0	92.6	0.0	0.0
Bromodichloromethane	1.1	0.0	0.2	0.0	98.7	0.0	0.0
Bromoform	7.1	0.0	1.2	0.1	83.7	8.0	0.0
Butyl benzyl phthalate	85.2	0.0	14.1	0.5	0.2	0.0	0.0
Chloroethane	0.0	0.0	0.0	0.0	100.0	0.0	0.0
Chloromethane	0.0	0.0	0.0	0.0	50.0	0.0	50.0
<i>Cis</i> 1,2 Dichloroethene	0.4	0.0	0.1	0.0	97.2	2.4	0.0
Dichloromethane	0.2	0.0	0.0	0.0	95.7	0.2	3.9
Diethyl Phthalate	64.2	0.0	10.6	0.4	24.2	0.6	0.0
Di- <i>n</i> -butyl phthalate	67.6	0.0	11.2	0.4	2.3	18.5	0.0
Di- <i>n</i> -octyl phthalate	80.2	0.0	13.3	0.5	0.0	6.0	0.0
Hexachloroethane	5.3	0.0	0.9	0.0	43.9	50.0	0.0
Isopropylbenzene	3.0	0.0	0.5	0.0	92.8	0.0	3.7
Methyl <i>tert</i> -butyl ether	1.5	0.0	0.3	0.0	97.8	0.0	0.4
Propylbenzene	4.7	0.0	0.8	0.0	94.4	0.0	0.1
Styrene	3.7	0.0	0.6	0.0	95.6	0.0	0.0
Total Cresols (2-, 3- and 4-methylphenol)	82.4	0.0	13.6	0.5	3.5	0.0	0.0
<i>Trans</i> 1,2 Dichloroethene	0.2	0.0	0.0	0.0	99.0	0.3	0.5
Tributyl tin oxide	42.6	0.0	7.0	0.3	0.5	49.6	0.0



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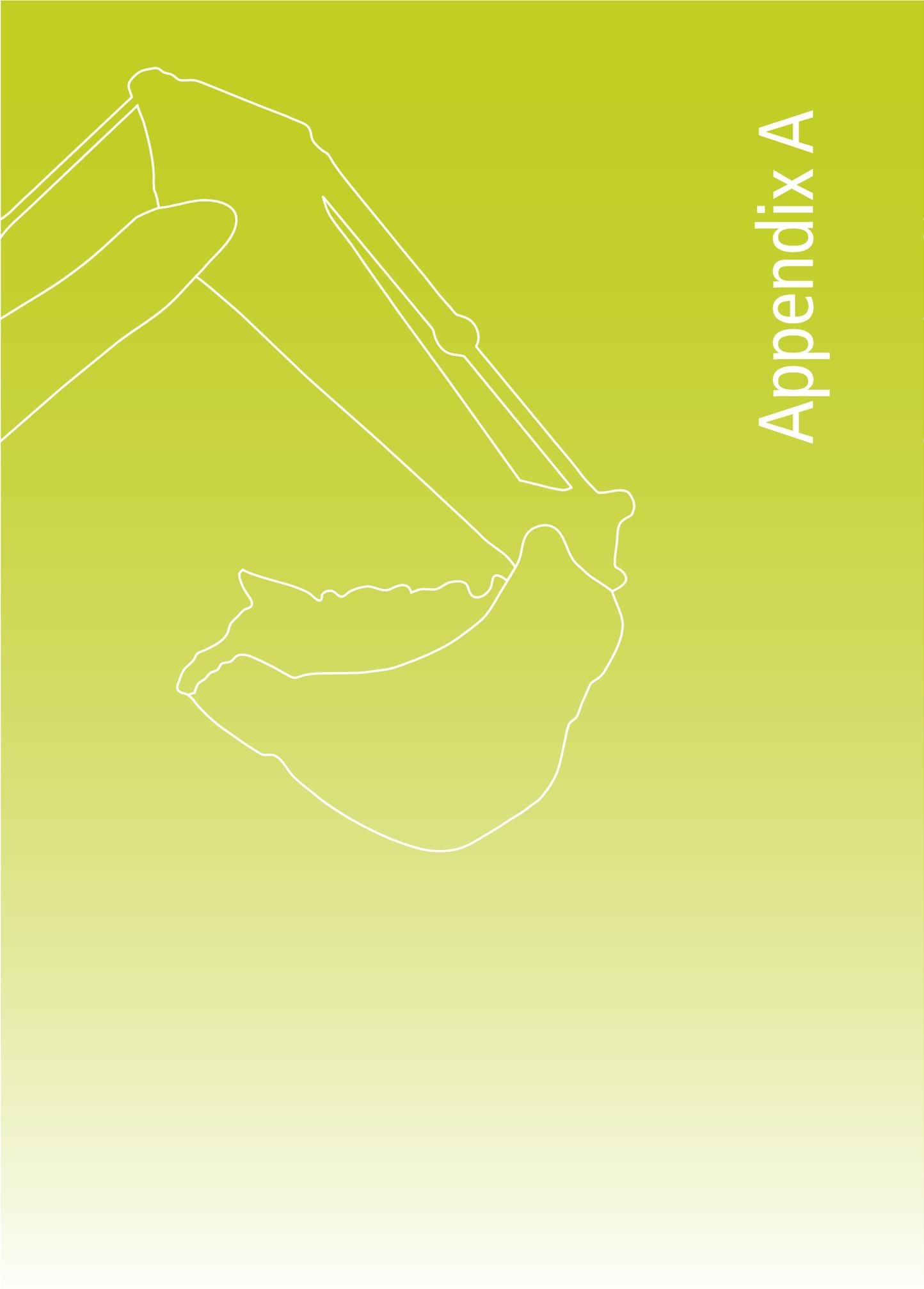
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# Appendix A

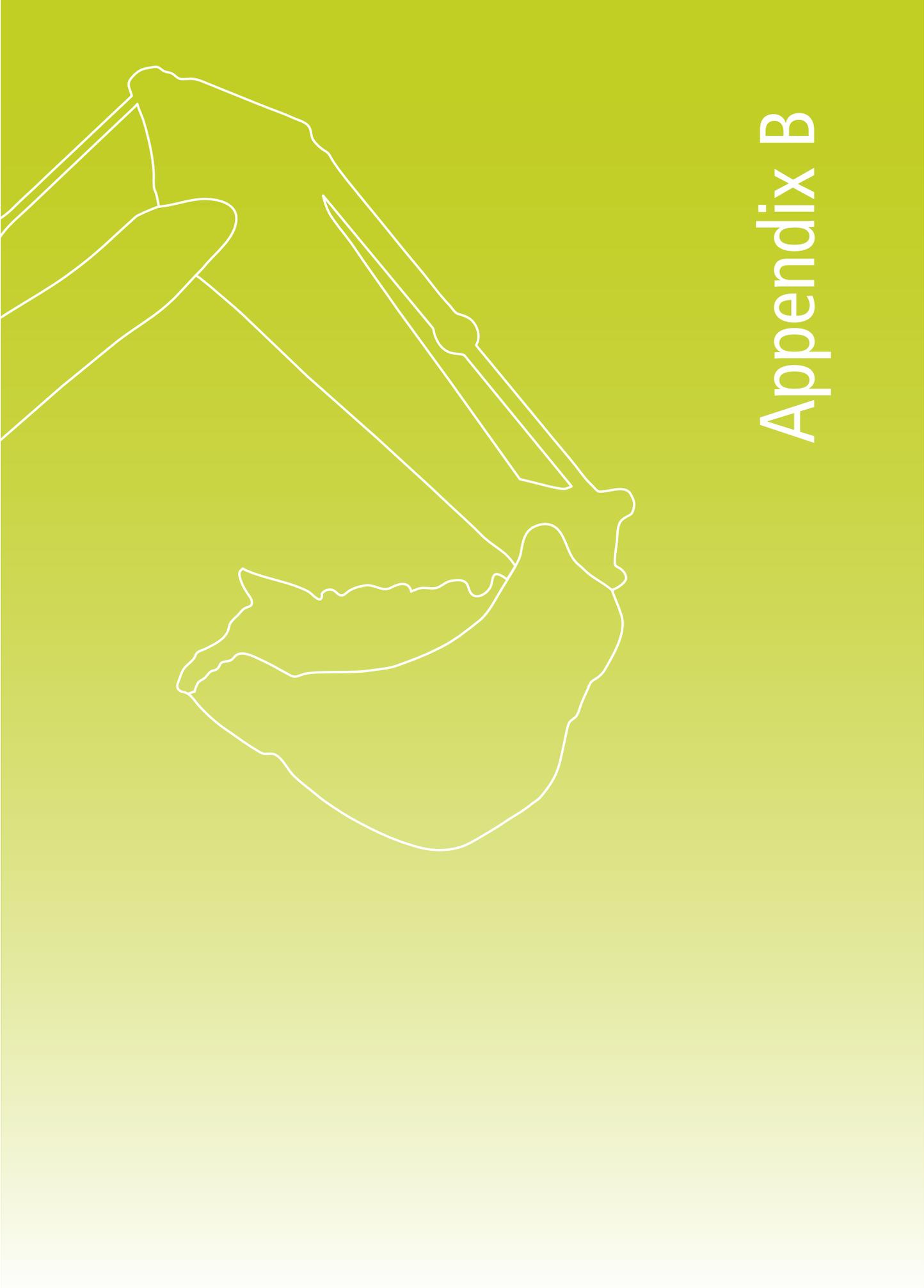
## Appendix A: Contaminant database CLEA inputs

Chemical	Oral HCV			Compare			Inhal HCV		Compare			Combine oral and inhalation AC	Oral MDI for adults	Inh MDI for adults	Air-water partition coefficient (Kaw)	Diffusion coefficient in air	Diffusion coefficient in water	Relative molecular mass	Vapour pressure	Water solubility	Organic carbon - water partition coefficient (Koc)	Octanol - water partition coefficient (Kow)	Soil water partition coefficient (Kd)	Dermal Absorption Factor	Soil-plant concentration factors	Soil-dust transport factor	Subsurface soil to indoor air correction factor
	Chemical type	Type	ug.kg-1.d-1	Oral	Derm	Inh	Type	ug.kg-1.d-1	Oral	Derm	Inh																
<sup>1</sup> Antimony	Inorganic	TDI	6	Yes	Yes	No	TDI	0.057	No	No	Yes	Yes	2.5	0.46	NR	NR	NR	NR	NR	987000	NR	NR		0		0.5	1
<sup>1</sup> Barium	Inorganic	TDI	20	Yes	Yes	Yes	NR		No	No	No	NR	847	1000	NR	NR	NR	NR	NR	800000	NR	NR		0		0.5	1
<sup>1</sup> Molybdenum	Inorganic	TDI	10	Yes	Yes	No	TDI	3.43	No	No	Yes	Yes	134.8	0	NR	NR	NR	NR	NR	840000	NR	NR		0		0.5	1
1,1,2-Trichloroethane	Organic	TDI	4	Yes	Yes	No	TDI	4.85	No	No	Yes	Yes	0.24	1	1.75E-02	7.58E-06	5.99E-10	133.4033	1386	4491	2.03	2.38	NR	0.1	Modelled	0.5	1
1,1-dichloroethane	Organic	TDI	200	Yes	Yes	Yes	NR		No	No	No	NR	20	4	1.29E-01	8.73E-06	6.74E-10	98.96	15452	3666	1.55	1.79	NR	0.1	Modelled	0.5	1
1,1-Dichloroethene	Organic	TDI	46	Yes	Yes	No	TDI	57	No	No	Yes	Yes	6	0.4	5.93E-01	9.18E-06	7.08E-10	96.9427	41983	3100	1.83	2.13	NR	0.1	Modelled	0.5	1
1,2,4-Trimethylbenzene	Organic	NR		No	No	No	TDI	2	Yes	Yes	Yes	Yes	24	86	8.56E-02	6.44E-06	4.87E-10	120.191	110	559	3.15	3.76	NR	0.1	Modelled	0.5	1
1,2-Dichloropropane	Organic	TDI	14	Yes	Yes	No	TDI	1.14	No	No	Yes	Yes	38	5.2	7.19E-02	7.74E-06	5.95E-10	112.99	3072	2050	1.71	1.99	NR	0.1	Modelled	0.5	1
<sup>2</sup> 1,3,5-Trimethylbenzene	Organic	NR		No	No	No	NR		No	No	No	No	8	20.5	1.19E-01	6.45E-06	4.87E-10	120.191	139	50	2.87	3.42	NR	0.1	Modelled	0.5	1
<sup>2</sup> 1-Methylnaphthalene	Organic	ID	2.3	Yes	Yes	No	NR	NR	No	No	No	NR	NR	NR	8.74E-03	6.02E-06	4.75E-10	142.2	2.97	20.5	3.23	3.87	NR	0.13	Modelled	0.5	1
2,4-Dimethylphenol	Organic	TDI	20	Yes	Yes	Yes	NR		No	No	No	NR	0	0	3.57E-04	6.56E-06	5.15E-10	122.16	5.28	8106	2.42	2.35	NR	0.1	Modelled	0.5	1
2,4-Dinitrotoluene	Organic	TDI	2	Yes	Yes	Yes	NR		No	No	No	No	0	0	3.67E-07	5.71E-06	4.66E-10	182.13	0.0154	129	2.15	1.98	NR	0.102	Modelled	0.5	1
2,6-Dinitrotoluene	Organic	TDI	1	Yes	Yes	Yes	NR		No	No	No	NR	0	0	1.57E-06	5.74E-06	4.66E-10	182.13	0.0372	232	2.22	2.1	NR	0.099	Modelled	0.5	1
2-Chloronaphthalene	Organic	TDI	80	Yes	Yes	No	TDI	0.286	No	No	Yes	Yes	0.0001	0.02	3.78E-03	5.95E-06	4.77E-10	162.62	0.501	11.7	3.32	3.98	NR	0.1	Modelled	0.5	1
<sup>2</sup> 2-Methylnaphthalene	Organic	TDI	4	Yes	Yes	No	NR	NR	No	No	No	NR	0	1	6.06E-03	6.03E-06	4.75E-10	142.2	3.41	25	3.34	4	NR	0.13	Modelled	0.5	1
2-Methylphenol	Organic	TDI	100	Yes	Yes	Yes	NR		No	No	No	NR	0	0.634	1.80E-05	7.17E-06	5.67E-10	108.138	15.3	12383	2.21	1.98	NR	0.1	Modelled	0.5	1
3-Methylphenol	Organic	TDI	100	Yes	Yes	Yes	NR		No	No	No	NR	0	0.634	1.04E-05	7.13E-06	5.67E-10	108.138	8.54	22500	2.2	1.97	NR	0.1	Modelled	0.5	1
4-Methylphenol	Organic	TDI	100	Yes	Yes	Yes	NR		No	No	No	NR	0	0.634	1.63E-05	7.13E-06	5.67E-10	108.138	8.54	23392	2.19	1.94	NR	0.1	Modelled	0.5	1
Biphenyl	Organic	TDI	38	Yes	Yes	Yes	NR		No	No	No	NR	4.49	0.524	5.78E-03	5.74E-06	4.51E-10	154.21	0.358	4.06	3.15	3.76	NR	0.1	Modelled	0.5	1
Bis (2-ethylhexyl) phthalate	Organic	TDI	50	Yes	Yes	Yes	NR		No	No	No	NR	300	15	3.90E-05	3.24E-06	2.44E-10	390.56	0.0001	0.27	3.74	5.63	NR	0.1	Modelled	0.5	1
Bromobenzene	Organic	TDI	24	Yes	Yes	No	TDI	3.43	No	No	Yes	Yes	0	0	3.10E-02	7.21E-06	5.85E-10	157.01	180.36	388.04	2.52	2.99	NR	0.1	Modelled	0.5	1
Bromodichloromethane	Organic	ID	0.3	Yes	Yes	Yes	NR		No	No	No	NR	NR	NR	3.19E-02	8.16E-06	6.70E-10	163.83	3788.674	3000	1.74	2.02	NR	0.1	Modelled	0.5	1
Bromoform	Organic	TDI	20	Yes	Yes	Yes	NR		No	No	No	NR	42	70	8.09E-03	7.56E-06	6.51E-10	252.73	305	3000	2.03	2.38	NR	0.1	Modelled	0.5	1
Butyl benzyl phthalate	Organic	TDI	500	Yes	Yes	Yes	NR		No	No	No	NR	8	0.04	5.26E-06	3.88E-06	3.01E-10	312	0.00015	2.32	3.28	4.65	NR	0.1	Modelled	0.5	1
<sup>2</sup> Carbazole	Organic	NR					NR					Yes			1.15E-03	5.39E-06	4.40E-10	167.21	7.64E-06	1.164	2.89	3.6	NR	0.1	Modelled	0.5	1
Chloroethane	Organic	NR		No	No	No	TDI	2857	Yes	Yes	Yes	NR	0	13.5	4.45E-01	1.05E-05	7.83E-10	64.51	93272	5742	1.27	1.44	NR	0.1	Modelled	0.5	1
Chloromethane	Organic	NR		No	No	No	TDI	5.14	Yes	Yes	Yes	NR	0	212	2.71E-01	1.28E-05	9.70E-10	50.488	330530.7	5350	0.84	0.91	NR	0.1	Modelled	0.5	1
Cis 1,2 Dichloroethene	Organic	TDI	6	Yes	Yes	Yes	NR		No	No	No	NR	4	6	7.46E-02	9.02E-06	7.08E-10	96.941	13685.66	7550	1.61	1.86	NR	0.1	Modelled	0.5	1
Dichloromethane	Organic	TDI	6	Yes	Yes	No	TDI	134.3	No	No	Yes	Yes	88.118	350	5.64E-02	9.97E-06	7.91E-10	84.93	31371	20080	1.14	1.28	NR	0.1	Modelled	0.5	1
Diethyl Phthalate	Organic	TDI	200	Yes	Yes	Yes	NR		No	No	No	Yes	80.5	2	2.64E-04	4.81E-06	3.75E-10	222.237	0.035	1200	2.15	2.25	NR	0.1	Modelled	0.5	1
<sup>2</sup> Dimethyl phthalate	Organic	NR					NR								1.58E-04	5.33E-06	4.23E-10	194.18	0.118109	4000	1.85	1.61	NR	0.1	Modelled	0.5	1
Di-n-butyl phthalate	Organic	TDI	10	Yes	Yes	No	TDI	10	No	No	Yes	No	133	0.12	3.00E-04	4.05E-06	3.12E-10	278.34	0.00114	13.3	3.24	4.57	NR	0.1	Modelled	0.5	1
Di-n-octyl phthalate	Organic	TDI	50	Yes	Yes	Yes	NR		No	No	No	NR	210	0.01	4.96E-12	3.24E-06	2.44E-10	390.56	9.74E-05	0.075831	4.87	8.04	NR	0.1	Modelled	0.5	1
Hexachloroethane	Organic	TDI	1	Yes	Yes	Yes	NR		No	No	No	Yes	14.02	86.44	1.31E-01	5.87E-06	4.63E-10	236.74	0.819	49.9	3.34	4	NR	0.1	Modelled	0.5	1
Iso-propylbenzene	Organic	TDI	100	Yes	Yes	No	TDI	114.3	No	No	Yes	Yes	0	294	2.37E-01	6.49E-06	4.87E-10	120.19	267	56	3.06	3.65	NR	0.1	Modelled	0.5	1
<sup>2</sup> Isopropyltoluene	Organic	NR		No	No	No	NR		No	No	No	NR	0	880	1.17E-01	6.02E-06	4.52E-10	134.218	80.9	51	3.42	4.1	NR	0.1	Modelled	0.5	1
Methyl tert-butyl ether	Organic	TDI	300	Yes	Yes	No	TDI	722	No	No	Yes	Yes	1	200	1.60E-02	7.82E-06	5.62E-10	88.1482	18425	48000	1.53	0.94	NR	0.1	Modelled	0.5	1
<sup>2</sup> n butylbenzene	Organic	NR		No	No	No	NR		No	No	No	No	0	5.4	1.86E-01	6.00E-06	4.52E-10	134.22	54.5	20.4	3.55	4.26	NR	0.1	Modelled	0.5	1
Propylbenzene	Organic	TDI	100	Yes	Yes	No	TDI	220	No	No	Yes	Yes	0	16.44	1.70E-01	6.35E-06	4.75E-10	120.19	180.06	54.1	3.09	3.69	NR	0.1	Modelled	0.5	1
<sup>2</sup> sec butylbenzene	Organic	NR		No	No	No	NR		No	No	No	No	0	5.4	2.76E-01	6.03E-06	4.52E-10	134.218	88.4	14	3.8	4.57	NR	0.1	Modelled	0.5	1
Styrene	Organic	TDI	12	Yes	Yes	No	TDI	240	No	No	Yes	Yes	1	5.6	5.33E-02	7.19E-06	5.48E-10	104.15	350	290	2.51	2.98	NR	0.1	Modelled	0.5	1
<sup>2</sup> tert butylbenzene	Organic	NR		No	No	No	NR		No	No	No	No	0	780	2.00E-01	6.04E-06	4.52E-10	134.218	144	27.3	3.43	4.11	NR	0.1	Modelled	0.5	1
Trans 1,2 Dichloroethene	Organic	TDI	17	Yes	Yes	No	TDI	17	No	No	Yes	Yes	4	6	1.77E-01	9.09E-06	7.08E-10	96.94	22569.71	5250	1.78	2.08	NR	0.1	Modelled	0.5	1
Tributyl tin oxide	Organic	TDI	0.25	Yes	Yes	No	TDI	0.0057	No	No	Yes	Yes	9	0	4.24E-05	3.25E-06	2.49E-10	596.11	0.000856	5.1	3.13	4.05	NR	0.1	Modelled	0.5	1

## Notes

1 Contaminants lack the necessary physico-chemical parameter values to derive GAC for land-uses involving plant uptake

2 Contaminants lack the necessary HCV to derive GAC



# Appendix B

Antimony	CAS Number:	7440-36-0	Assessor A:	Andreas Neymeyer, Buro Happold	Assessor B:	Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF
	Date	16/04/2009	Date	16/04/2009	Date	26/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	No data to indicate carcinogenicity by the oral route. TDI oral applied to oral and dermal exposures.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		Some evidence for the carcinogenicity of certain antimony compounds by inhalation; however, no data to derive a health criteria value for cancer risk. TDlinh applied to inhalation exposures.

TDI oral	Recommended TDloral	Units	Justification
	6	ug.kg-1.d-1	TDI as suggested by the WHO and FSA. Note that the lower Health Canada value (0.2ug.kg-1.d-1) is based on a NOAEL of 0.06 mg/kg of body weight per day proposed by Poon et al. (1998). This NOAEL was questioned by Lynch et al. (1999) who preferred a NOAEL of 6.0 mg/kg of body weight per day, which has subsequently been used by the WHO and FSA.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description	Target organ/Critical Effect	
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	2003	27/03/2009	TDI		6 µg/kg bw/day	6		NOAEL		6 mg/kg body weight per day		1000	100 for inter- and intraspecies variation, 10 for the short duration of the study	animal (rats)	Effects of antimony on rats following 90-day exposure via drinking water	Animal studies: decreased longevity and altered blood levels of glucose and cholesterol, reversible loss of body weight gain, <b>subtle histopathological changes in thyroids</b> (increased epithelial height, decreased follicular size)  Humans: vomiting, nausea, abdominal cramps and diarrhoea, optic nerve destruction, uveitides and retinal bleeding, accompanied by headache, coughing, anorexia, troubled sleep and vertigo Antimony-containing compounds may also produce alterations in cardiac function and autopsy studies have shown that cardiac toxicity was the cause of death in patients treated with antimonal drugs. There is no information on the oral carcinogenicity of antimony and compounds in humans. However based on inhalation data in rats and in vitro data, the IARC concluded that antimony trioxide is possibly carcinogenic to humans (Group 2B), and antimony trisulfide is not classifiable as to its carcinogenicity to humans (Group 3)
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2003	27/03/2009	TDI		6 µg/kg bw/day	6		NOAEL		6 mg/kg body weight per day		1000	100 for inter- and intraspecies variation, 10 for the short duration of the study	animal (rats)	Effects of antimony on rats following 90-day exposure via drinking water	
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	Aug 1999	27/03/2009	TDI	0.0002	mg/kg body weight per day	0.2	3	NOAEL	0.06	mg/kg body weight per day		300	x10 for intraspecies variation; x10 for interspecies variation; and x3 for the use of a short-term study	animal (rats)	Effects of antimony on rats following 90-day exposure via drinking water	

TDI inhal	Recommended TDlinhal	Units	Justification
	0.057		Health criteria calculated from RFC as suggested by IRIS. Calculation performed in line with SC050021/SR2

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description	Response	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	09/01/1995	12/08/2009	RFC	0.0002	mg/m <sup>3</sup>	0.057	Medium	Study & Database	0.07	mg/kg body weight per day		300	An uncertainty factor of 10 is used for the protection of sensitive human subpopulations, 3 is used for interspecies extrapolation because the dosimetric adjustments account for part of this area of uncertainty, 3 is applied for database inadequacies. An additional threefold uncertainty factor to account for a less-than-lifetime exposure duration is applied. This is less than the 10-fold uncertainty factor normally applied to adjust from subchronic (90-day) to chronic studies because exposures lasted for 1 full year.	animal (rats)	Chronic study in which groups of rats were exposed to target concentrations of 0, 0.05, 0.50, or 5.00 mg/m <sup>3</sup> antimony trioxide for 6 hours/day, 5 days/week for 1 year.	"Microscopic lesions of the lungs revealed <b>interstitial inflammation</b> in control and exposure groups at the end of 6, 12, 18, and 24 months. <b>Granulomatous inflammation and granulomas</b> were observed in all exposure groups at 18 and 24 months. An increase in the number of alveolar and intraalveolar particle-laden macrophages was observed (at every exposure duration) in all but the control groups."
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>				"Although there is some evidence for the carcinogenicity of certain antimony compounds by inhalation, there are no data to indicate carcinogenicity by the oral route." There also appears to be no data available to derive a guidance value for inhalation exposure.												

ID oral	Recommended IDoral	Units	Justification
	n/a		Although there is some evidence for the carcinogenicity of certain antimony compounds by inhalation, there is no data to indicate carcinogenicity by the oral route.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type	Description	Response
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ID inhal	Recommended IDinhal	Units	Justification
	n/a		No data for inhalation Index Dose

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type	Description	Response
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Antimony

TDI oral
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Organisation	Reference	Web link
Food Standards Agency (FSA)	Poon et al. 1998 & Lynch et al. 1999	<a href="http://cot.food.gov.uk/pdfs/TOX-2003-39.PDF">http://cot.food.gov.uk/pdfs/TOX-2003-39.PDF</a>
WHO Guidelines for drinking water Quality	Poon et al. 1998 & Lynch et al. 1999	<a href="http://www.who.int/water_sanitation_health/dwa/chemicals/antimony.pdf">http://www.who.int/water_sanitation_health/dwa/chemicals/antimony.pdf</a>
Health Canada Toxicological Values	Poon et al. 1998	<a href="http://www.hc-sc.gc.ca/ewh-semt/eubs/water-eau/antimony-antimoine/classification-eng.php">http://www.hc-sc.gc.ca/ewh-semt/eubs/water-eau/antimony-antimoine/classification-eng.php</a>

TDI inhal
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Organisation	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	Newton et al. 1994, Muhle et al. 1990	<a href="http://www.epa.gov/ncea/iris/subst/0676.htm#inhalrhc">http://www.epa.gov/ncea/iris/subst/0676.htm#inhalrhc</a>
WHO Guidelines for drinking water Quality	IARC. 1989. Some organic solvents, resin monomers and related compounds, pigments and occupational exposures in paint manufacture and painting. Lyon, International Agency for Research on Cancer, pp. 291–305 (IARC Monographs on the Evaluation of Carcinogenic Risks to Humans, Vol. 47 in WHO. 2003. Antimony in Drinking-water - Background document for development of WHO Guidelines for Drinking-water Quality	<a href="http://www.who.int/water_sanitation_health/dwa/chemicals/antimony.pdf">http://www.who.int/water_sanitation_health/dwa/chemicals/antimony.pdf</a>

ID oral
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Organisation	Reference	Web link
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ID inhal
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Organisation	Reference	Web link
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Antimony	CAS 7440-36-0	Assessor A: Andreas Neymeyer, Buro Happold	Assessor B: Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF	
	Date	09/04/2009	Date	09/04/2009	Date	26/08/2009

MDI			Recommended MDI <sub>oral</sub>	Units	Justification: UK population estimate of dietary intake from FSA 2006 total diet study		
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Food Standards Agency (FSA)	Jan-09	food	2.5	µg day <sup>-1</sup>	Estimate of population dietary intake from total food survey of 20 food groups from 24 UK towns	FSA, 2009. Measurement of the concentrations of metals and other elements from the 2006 UK total diet study	<a href="http://www.food.gov.uk/multimedia/pdfs/fsis0909metals.pdf">http://www.food.gov.uk/multimedia/pdfs/fsis0909metals.pdf</a>
European Food Safety Authority (EFSA)	27/03/2009	food	42	µg day <sup>-1</sup>	A Restriction of 0.04 mg/kg of food (as Sb) is applied. This restriction would allow for 10% of the TDI being allocated to food contact materials.  TDI 6ug/kg(bw)/dayx70kg(bw)=420ug/day x 10% = 42ug/day	The EFSA Journal (2004) 24, 1-13 , Opinion of the Scientific Panel on food additives, flavourings, processing aids and materials in contact with food (AFC) on a request from the Commission related to a 2nd list of substances for food contact materials. ( <a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/opinion_afc_06_en1,0.pdf">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/opinion_afc_06_en1,0.pdf</a> )	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a>
WHO Guidelines for Drinking Water Quality	27/03/2009	water [assuming 5µg/l in drinking water and 2l water consumption]]	10	µg day <sup>-1</sup>	"The concentrations in drinking-water appear to be less than 5 µg/litre" (also note: UK Drinking Water Standards (DWS) for antimony = 5ug day <sup>-1</sup> )"	US EPA, 1984; Longtin, 1985 ( <a href="http://www.who.int/water_sanitation_health/dwq/chemicals/antimony.pdf">http://www.who.int/water_sanitation_health/dwq/chemicals/antimony.pdf</a> )	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">www.who.int/water_sanitation_health/dwq/guidelines/en</a>
WHO Guidelines for Drinking Water Quality	27/03/2009	oral total	70	µg day <sup>-1</sup>	Daily oral uptake of antimony ranges from 10 to 70 µg	Gebel T. 1999. Metalle/Antimon. In: Wichmann-Schlipkötter-Fülgraff, eds. Umweltmedizinisches Handbuch, 17. Ergänzungslieferung (November 1999). Landsberg, ecomed. ( <a href="http://www.who.int/water_sanitation_health/dwq/chemicals/antimony.pdf">http://www.who.int/water_sanitation_health/dwq/chemicals/antimony.pdf</a> )	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">www.who.int/water_sanitation_health/dwq/guidelines/en</a>
International Antimony Oxide Industry Association	27/03/2009	oral total	70	µg day <sup>-1</sup>	The daily intake from food and water ranges from to 10 to 70 micrograms (µg) per day.	Antimony Trioxide Frequently Asked Questions: March 2006 ( <a href="http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf">http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf</a> )	<a href="http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf">http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf</a>
MDI			Recommended MDI <sub>inh</sub>	Units	Justification: As reported in Slooff W (1992) Exploratory report. Antimony and antimony compounds. Bilthoven, Rijksinstituut voor de Volksgezondheid en Milieuhygiene.		
Organisation	Date	Media	Value	Units	Description	Reference	Web link
WHO Guidelines for Drinking Water Quality	27/03/2009	Air	0.46	µg day <sup>-1</sup>	Exposure of the typical urban population to antimony from air is estimated to be between 60 and 460 ng/day per person	Slooff W (1992) Exploratory report. Antimony and antimony compounds. Bilthoven, Rijksinstituut voor de Volksgezondheid en Milieuhygiene.	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">www.who.int/water_sanitation_health/dwq/guidelines/en</a>
International Antimony Oxide Industry Association	27/03/2009	Air	0.15	µg day <sup>-1</sup>	The main sources of antimony in urban air are from industrial dust, car emissions and fuel oil combustion, but still are very low (0.15ug/kg/day).	Antimony Trioxide Frequently Asked Questions: March 2006 ( <a href="http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf">http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf</a> )	<a href="http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf">http://www.nihonseiko.co.jp/english/environment/060418faq_e.pdf</a>



Barium	CAS Number:	7440-39-3	Assessor A:	Cheryl Davies, Delta-Simons	Assessor B:	Jennifer Stothert, Entec UK Ltd	Final review:	Panel/SF
	Date	27/03/2009	Date	29/04/2009	Date	25/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDioral to exposure routes?	Yes	Yes	Yes	NR	Insufficient data to assess non threshold effects - so HCV based on threshold effects. Insufficient data to assess non threshold effects - so HCV based on threshold effects. Insufficient data with sufficient detail on derivation to derive HCVinh, use route to route extrapolation from oral HCV
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDioral	Units	Justification
	20	ug.kg-1.d-1	FSA, COT, CICADs recommendation

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	01/11/2008	27/03/2009	TDI oral	20	ug.kg bw-1.d-1	20		NOAEL	0.21	mg.kg bw-1.d-1		10 to allow for database deficiencies and differences between humans	Short term	11 healthy male volunteers were administered drinking water containing barium chloride ( 0 mg/l for 2 weeks, 5 mg/l for the next 4 weeks and 10 mg/l for the last 4 weeks)
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	Draft 2008	27/03/2009	TDI oral (same data as FSA)	20	ug.kg bw-1.d-1	20	Draft Report	NOAEL	0.21	mg.kg bw-1.d-1		10 to allow for database deficiencies and differences between humans	Short term	11 healthy male volunteers were administered drinking water containing barium chloride ( 0 mg/l for 2 weeks, 5 mg/l for the next 4 weeks and 10 mg/l for the last 4 weeks)
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://incem.org/pages/cicads.html">http://incem.org/pages/cicads.html</a>	2001	27/03/2009	TDI oral	0.02	mg.kg bw-1.d-1	20	The use of a NOAEL from human studies increases the confidence in the derivation of the TDI. The overall confidence is medium, reflecting medium confidence in the principal studies and in the database.	NOAEL	0.21	mg.kg bw-1.d-1		10 to allow for database deficiencies and differences between humans	Short term	Wones et al. (1990) administered 1.5 litres/day of distilled drinking-water containing various levels of barium chloride to 11 healthy male volunteers aged 27-61 years (mean 39.5 years, median 41 years). Barium concentrations in the drinking-water consumed by the subjects prior to the study were known to be very low. No barium was added for the first 2 weeks, which served as a control period; drinking-water containing 5 mg barium/litre (0.14 mg barium/kg body weight per day using reference values of 2 litres/day for water consumption and 70 kg for body weight) was administered for the next 4 weeks, and drinking-water containing 10 mg barium/litre (0.21 mg barium/kg body weight per day) was administered for the last 4 weeks of the study. Diets were controlled to mimic US dietary practices. Systolic & diastolic blood pressures were measured in the morning and evening. Blood was collected at the beginning and periodically. Twenty-four-hour urine collections were performed at the end of each study period.
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	<a href="http://incem.org/pages/sids.html">http://incem.org/pages/sids.html</a>	01/07/1999	27/03/2009	Information on C.I. Pigment Red 53:1 D and C red No. 9											
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/12/1992	27/03/2009	No HCV					Lowest chronic NOEC	2900	ug.l-1			Chronic toxicity	Toxicity study of freshwater organisms
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	12/09/2008	03/04/2009	Maximum Acceptable Concentration MAC in drinking water	1	mg.l-1	28.57	(Rounded up from 0.73 mg.l-1)	NOAEL	7.3	mg.l-1		10 Intraspecies variation	Epidemiological study	Epidemiological study of population ingesting water containing Ba
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	01/08/2007	26/03/2009	MRL	0.2	mg.kg bw-1.d-1	200		BMDL5	61.13	mg.kg bw-1.d-1		10 for extrapolation of animals to humans 10 for human variability 3 for database deficiencies	Chronic oral study	Mouse study. Groups of 60 male and 60 female B6C3F1 mice were administered 0, 500, 1,250, or 2,500 ppm barium chloride dehydrate in drinking water for 2 years. Using measured body weights and water consumption, the investigators estimated the daily barium doses to be 0, 30, 75, and 160 mg barium/kg/day for males and 0, 40, 90, and 200 mg barium/kg/day for females.
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Summer 2006	08/04/2009	RD in drinking water for Child	0.2	mg.kg-1.d-1	200								Data is from Iris
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	11/07/2005	08/04/2009	Oral RfD	0.2	mg.kg-1.d-1	200	Medium	BMD 05 BMDL 05	84 63	mg.kg-1.d-1 mg.kg-1.d-1		10 for extrapolation for interspecies differences (UFA: animal to human); 10 for consideration of intraspecies variation (UFH: human variability); and 3 for deficiencies in the database (UFD).	Chronic and subchronic oral	NTP (1994) exposed both sexes of F344/N rats and both sexes of B6C3F1 mice to barium chloride dihydrate (BaCl2x2H2O) in drinking water for 13 weeks or 2 years. Drinking water concentrations in the chronic study (60 animals/sex/group) were and 0, 500, 1250, and 2500 ppm. The study authors estimated doses, using water consumption and body weight data, as 0, 15, 30, and 60 mg Ba/kg-day for male rats and 0, 15, 45, and 75 mg Ba/kg-day for female rats. The estimated doses for mice were 30, 75, and 160 mg Ba/kg-day for males and 40, 90, and 200 mg Ba/kg-day for females. In the subchronic study (10 animals/sex/group), drinking water concentrations were 0, 125, 500, 1000, 2000, and 4000 ppm. Estimated doses were 0, 10, 30, 65, 110, and 200 mg Ba/kg-day for male rats and 0, 10, 35, 65, 115, and 180 mg Ba/kg-day for female rats. For mice, the corresponding estimated doses were 0, 15, 55, 100, 205, and 450 mg Ba/kg-day for the males and 0, 15, 60, 110, 200, and 495 mg Ba/kg-day for the females. The animals were fed an NIH-07 diet. Barium was not reported as a contaminant of the feed.

Barium

TDI oral			
Organisation	Target organ/Critical Effect	Reference	Web link
Food Standards Agency (FSA)	No effects	WHO (2001b). Concise International Chemical Assessment Document 33: Barium and barium compounds. World Health Organization, Geneva. In COT 2006 UK Total diet study of metals and other elements	<a href="http://cot.food.gov.uk/pdfs/tox200837.pdf">http://cot.food.gov.uk/pdfs/tox200837.pdf</a>
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	No effects	WHO (2001b). Concise International Chemical Assessment Document 33: Barium and barium compounds. World Health Organization, Geneva. In COT 2006 UK Total diet study of metals and other elements	<a href="http://cot.food.gov.uk/pdfs/tox200837.pdf">http://cot.food.gov.uk/pdfs/tox200837.pdf</a>
IPCS concise International Chemical Assessment Documents (CICADs)	This study did not identify a LOAEL	Wones RG, Stadler BL, Frohman LA (1990) Lack of effect of drinking water barium on cardiovascular risk factors. Environmental health perspectives, 85:1-13. Within Concise International Chemical Assessment Document 33 Barium and Barium Compounds, WHO, Geneva 2001	<a href="http://incchem.org/documents/cicads/cicads/cicad33.htm">http://incchem.org/documents/cicads/cicads/cicad33.htm</a>
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals		<a href="http://www.inchem.org/documents/sids/sids/5160021.pdf">http://www.inchem.org/documents/sids/sids/5160021.pdf</a>	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.		Towards integrated environmental quality objectives for surface water, ground water, sediment and soil for nine trace metals Plassche EJ van de, Bruijn JHM de RIVM Rapport 679101005	<a href="http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf">http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf</a>
Health Canada Toxicological Values	No adverse effects on blood pressure or cardiovascular disease	Brenniman, G.R. and Levy, P.S. Epidemiological study in Illinois drinking water supplies. In: Advances in modern environmental toxicology. Vol. IX. Princeton Publishing Co., Princeton, NJ. p. 231 (1985).	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/barium-baryum/index-eng.php#Health">http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/barium-baryum/index-eng.php#Health</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Moderate to marked severity nephropathy, which resulted in marked weight loss and increased mortality.	NTP. 1994. Toxicology and carcinogenesis studies of barium chloride dihydrate (CAS No. 10326-27-9) in F344/N rats and B6C3F1 mice (drinking water studies). U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program, Research Triangle Park, NC. NTP TR 432.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp24.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp24.pdf</a>
USEPA Health Advisors		US EPA Drinking Water Standards and Health Advisories, 2006	<a href="http://www.epa.gov/waterscience/criteria/drinking/dwstandards.html#inorganics">http://www.epa.gov/waterscience/criteria/drinking/dwstandards.html#inorganics</a>
USEPA Integrated Risk Information System (IRIS)	Chemical-related nephropathy was observed in male and female mice following chronic or subchronic drinking water exposure to barium chloride. These lesions were characterized by tubule dilatation, renal tubule atrophy, tubule cell regeneration, hyaline cast formation, multifocal interstitial fibrosis, and the presence of crystals, primarily in the lumen of the renal tubules.	National Toxicology Program (NTP). (1994) Technical report on the toxicology and carcinogenesis studies of barium chloride dihydrate (CAS No. 10326-27-9) in F344/N rats and B6C3F1 mice (drinking water studies). NTP TR 432. National Toxicological Program, Research Triangle Park, NC. NIH Pub. No. 94-3163. NTIS Pub PB94-214178.	<a href="http://www.epa.gov/ncea/iris/subst/0010.htm">http://www.epa.gov/ncea/iris/subst/0010.htm</a>

Barium		CAS Number:	7440-39-3		Assessor A:	Cheryl Davies, Delta-Simons		Assessor B:	Jennifer Stothert, Entec UK Ltd		Final review:	Panel/SF			
					Date	27/03/2009		Date	29/04/2009		Date	25/08/2009			
TDI inhal					Recommended TDI <sub>inhal</sub>			Units			Justification	Insufficient data with sufficient detail on derivation to derive			
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
IPCS concise International Chemical Assessment Documents (CIADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	01/12/2001	27/03/2009	The deficient reporting of the methods and results of the only											
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1990	27/03/2009	No pertinent data regarding chronic inhalation exposure to											
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/12/1992	27/03/2009	No HCV										Chronic toxicity	Toxicity study of freshwater organisms
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	11/07/2005	08/04/2009	An RFC for barium is not recommended at this time. The											
ID oral					Recommended ID <sub>oral</sub>			Units			Justification	Insufficient data			
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis		Study type	Description
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	22/08/1997	29/04/2009	Data only for D&C RED No. 9 (CI Pigment Red 53:1) - a barium salt. D&C Red No. 9 is not classifiable as to its carcinogenicity to humans (Group 3)											
IPCS concise International Chemical Assessment Documents (CIADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	2001	29/04/2009	There is a limited amount of information available on the genotoxicity of barium compounds. No in vivo studies have been conducted. Most in vitro studies have found that barium chloride and barium nitrate did not induce gene mutations in bacterial assays with or without metabolic activation.											
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1990	29/04/2009	The International Agency for Research on Cancer Working Group (IARC, 1980) evaluated the carcinogenicity of barium chromate (VI) and concluded that it is a positive human carcinogen. The carcinogenic property of this compound, however, has been ascribed to the chromium (VI) moiety and not to the barium.											
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/12/1992	29/04/2009	No HCV										Chronic toxicity	Toxicity study of freshwater organisms
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	01/08/2007	29/04/2009	Generally negative results in genotoxicity studies. Insufficient data for assessment											
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	11/07/2005	29/04/2009	The results of the oral carcinogenicity study suggest that barium is not likely to be carcinogenic to humans.											
ID inhal					Recommended ID <sub>inhal</sub>			Units			Justification	Insufficient data			
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis		Study type	Description
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/12/1992	29/04/2009											Chronic toxicity	Toxicity study of freshwater organisms

Barium

TDI inhal

Organisation	Response	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)	Studies suggest that the respiratory system is a target of barium toxicity.	Muller K (1973) Radiographic and morphological structural analyses for the differential diagnosis of chronic bronchitis and mild silicosis. Beitrage zur	<a href="http://inchem.org/documents/cicads/cicads/cicad33.htm#4.0">http://inchem.org/documents/cicads/cicads/cicad33.htm#4.0</a>
IPCS Environmental Health Criteria (EHC) Monographs			<a href="http://inchem.org/documents/ehc/ehc/ehc107.htm">http://inchem.org/documents/ehc/ehc/ehc107.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			<a href="http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf">http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf</a>
USEPA Integrated Risk Information System (IRIS)			

ID oral

Organisation	Response	Reference	Web link
International Agency for Research on Cancer (IARC)			<a href="http://www.inchem.org/documents/iarc/vol57/10-dcr9.html">http://www.inchem.org/documents/iarc/vol57/10-dcr9.html</a>
IPCS concise International Chemical Assessment Documents (CICADs)			
IPCS Environmental Health Criteria (EHC) Monographs			<a href="http://inchem.org/documents/ehc/ehc/ehc107.htm">http://inchem.org/documents/ehc/ehc/ehc107.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			<a href="http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf">http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels			<a href="http://www.atsdr.cdc.gov/toxprofiles/tp24.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp24.pdf</a>
USEPA Integrated Risk Information System (IRIS)			

ID inhal

Organisation	Response	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			<a href="http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf">http://www.rivm.nl/bibliotheek/rapporten/679101005.pdf</a>

Barium	CAS 7440-39-3	Assessor A: Date	Cheryl Davies 27/03/2009	Assessor B: Date	Sian Jones 29/04/2009	Final review: Date	Panel/SF 25/08/2009
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MDI	Recommended MDI oral	Units	Justification: UK population estimate of dietary intake from FSA 2006 total diet study
	847	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Drinking Water Inspectorate	28/11/1996	Surface waters	1000	ug l-1	For waters classified as DW2 or DW3 (MDI equivalent to 2000ug/day)	Surface Waters (Abstraction for Drinking water)(classification) regulations 1996	<a href="http://www.dwi.gov.uk">www.dwi.gov.uk</a>
Food Standards Agency (FSA)	Jan-09	food	847	µg day-1	Estimate of population dietary intake from total food survey of 20 food groups from 24 UK towns	FSA, 2009. Measurement of the concentrations of metals and other elements from the 2006 UK total diet study	<a href="http://www.food.gov.uk/multimedia/pdfs/fsis0909metals.pdf">http://www.food.gov.uk/multimedia/pdfs/fsis0909metals.pdf</a>
Committee on the Medical Effects of Air Pollutants (COMEAP)	//1998				The chemical form of the element in food is unknown. The relevance of the available toxicity data is therefore uncertain	<a href="http://www.advisorybodies.doh.gov.uk/coc/1998ar.pdf">http://www.advisorybodies.doh.gov.uk/coc/1998ar.pdf</a>	<a href="http://www.advisorybodies.doh.gov.uk/comeap/index.htm">www.advisorybodies.doh.gov.uk/comeap/index.htm</a>
European Food Safety Authority (EFSA)	//2008	Food			There are restrictions on the barium content of packaging in contact with food	<a href="http://ec.europa.eu/food/food/chemicalsafety/foodcontact/eu_substances_en.pdf">http://ec.europa.eu/food/food/chemicalsafety/foodcontact/eu_substances_en.pdf</a>	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a>
International Agency for Research on Cancer (IARC)	22/08/1997				Only data relating to Ba is for Barium chromate and D+C red no.9 (a sulphonic acid and barium salt mix)		<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>
IPCS INCHEM		Total daily intake	1326	ug.day-1	In the United Kingdom (Wales), the average dietary intake has been estimated to be 1240 µg/day and drinking water intake of 86 ug/day.		<a href="http://inchem.org/">http://inchem.org/</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	//2001	Daily dietary intake (food and drink)	0.3	mg.day-1	Median daily Intake of Ba for adults of 0.30 mg per person, between 1970 and 1991. Min is 0.18 and max is 0.72 (Equivalent MDI of 720ug/day)	WHO (1996) Guidelines for drinking-water quality, 2nd ed. Vol. 2. Health criteria and other supporting information. Geneva, World Health Organization. within CICAD 33, Barium and Barium Compounds, WHO, Geneva, 2001	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
IPCS Environmental Health Criteria (EHC) Monographs	//1990	Total daily intake	1327	ug.day-1	The estimated total daily intake of barium in Wales (United Kingdom) is 1327 µg (food 1240 µg; drinking- water 86 µg; air 1 µg).	Possibly from MORTON, M.S., ELWOOD, P.C., & AVERNETHY, M. (1976) Trace elements in water and congenital malformations of the central nervous system in South Wales. Br. J. Soc. Med., 30: 36-39. within EHC 107, 1990. WHO. Geneva.	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>
WHO Guidelines for Drinking Water Quality	//2004	Drinking water	0.7	mg.l-1	Guideline for drinking water quality (equivalent MDI of 1400ug/day)	WHO (1996) Guidelines for drinking-water quality, 3rd ed. Guideline values for chemicals that are of health significance in drinking water. Geneva, World Health Organization.	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">www.who.int/water_sanitation_health/dwq/guidelines/en</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	//1992	Drinking water	500	ug.l-1	Drinking water Environmental quality objective (Equivalent MDI of 1000ug/day)	Towards integrated environmental quality objectives for surface water, ground water, sediment and soil for nine trace metals Plassche EJ van de, Bruijn JHM de RIVM Rapport 679101005	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>

Barium		CAS 7440-39-3		Assessor A:	Cheryl Davies	Assessor B:	Sian Jones <th>Final review:</th> <td>Panel/SF</td>	Final review:	Panel/SF
		Date	27/03/2009	Date	29/04/2009	Date	25/08/2009		
Health Canada Toxicological Reference Values	02/04/2009	Food, drinking water and air	1	mg.d-1	mean daily intake of barium from food, water and air in Canada is estimated to be slightly more than 1 mg/d. Of this, food represents the primary source of barium for the non-occupationally exposed Canadian population. However, in cases where barium levels in drinking water are high (0.6 mg/L), drinking water may contribute significantly to barium intake (approximately 50%). [equivalent MDI of 1000ug/day]	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/barium-baryum/index-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/barium-baryum/index-eng.php</a>	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>		
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	10/05/2007	Drinking water	2	mg. L-1	US EPA Drinking water limit (equivalent MDI of 4000ug/day)	<a href="http://www.atsdr.cdc.gov/toxpro/files/tp24.html">http://www.atsdr.cdc.gov/toxpro/files/tp24.html</a>	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>		

Barium	CAS 7440-39-3	Assessor A:	Cheryl Davies	Assessor B:	Sian Jones	Final review:	Panel/SF
		Date	27/03/2009	Date	29/04/2009	Date	25/08/2009

MDI			Recommended MDI <sub>inh</sub>	Units	Justification: Upper limit reported by Tabor and Warren (1958) is within range reported by USEPA (1984) (both cited in IPCS CICADs) and has been converted to an MDI by multiplying by 20 m <sup>3</sup> /d and 1000 ug/mg.
			1000	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Health Protection Agency	//2005	Air	0.5	mg.m-3	Occupational exposure limit to Ba compounds soluble (as Ba). Long term exposure limit (8 hr TWA)	EH 40/2005, as consolidated with amendments October 2007 <a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>	<a href="http://www.hpa.org.uk">www.hpa.org.uk</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	//2001	Ambient air	0.05	mg.m-3	Levels of Ba in air generally rarely exceed 0.05 mg/m <sup>3</sup> (Tabor +Warren, 1958). In a more recent survey in the USA, ambient barium concentrations ranged from 0.0015 to 0.95 mg/m <sup>3</sup> (US EPA, 1984).	Tabor EC, Warren WV (1958) Distribution of certain metals in the atmosphere of some American cities. Archives of industrial health, 17:145-151 and US EPA (1984) Health effects assessment for barium. Prepared for the Office of Emergency and Remedial Response, US Environmental Protection Agency, Washington, DC. Cincinnati, OH, US Environmental Protection Agency, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office (EPA540/1-86-021), within CICAD 33, Barium and Barium Compounds, WHO, Geneva, 2001	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
IPCS Environmental Health Criteria (EHC) Monographs	//1990	Ambient air	The intake via inhalation is estimated to range from 0.04 to 3.1 µg/day.	ug/day	Concentrations measured in air in US of 0.0015 to 0.95 ug.m-1	US EPA (1984) Health effects assessment for barium, Cincinnati, Ohio, US Environmental Protection Agency, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office (Prepared for the Office of Emergency and Remedial Response, Washington, DC) (EPA 540/1-86-021).  EHC 107, 1990. WHO. Geneva.	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	01-Aug-07	Workplace Air	0.5	mg.m-3	US NIOSH Recommended Exposure limit in workplace air 8 hr	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp24.html">http://www.atsdr.cdc.gov/toxprofiles/tp24.html</a>	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>



Molybdenum	CAS Number:	7439-98-7	Assessor A:	Nick Struggles, AECOM	Assessor B:	Atkins	Final review:	Penl/SF
	Date:	01/06/2009	Date:	17/06/2009	Date:	26/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Insufficient data to assess non threshold effects - so HCV based on threshold effects. TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	10	ug.kg-1.d-1	Recommended by EFSA and RIVM. Both studies are more recent than the USEPA (which had a lower value).

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
European Food Safety Authority (EFSA)	<a href="http://www.efsa.europa.eu/en.html">http://www.efsa.europa.eu/en.html</a>	01/02/2006	01/06/2009	TDI oral	0.01	mg/kg bw/day	10	Medium	NOAEL	0.9	mg/kg bw/day	100	10 for protecting sensitive human sub-populations with inadequate Cu intake or with deficient Cu metabolism in view of the species differences in antagonism between Mo and Cu, and another factor of 10 to cover the lack of knowledge about reproductive effects of Mo in humans and incomplete data on the toxicokinetics in man.	9 week study of rats (diet and drinking water)	A tolerable upper intake level (UL) can be established using the 9-week study in the rat (Fungwe et al, 1990). a) is the tolerable upper intake level b) is equivalent for adults  5 groups, each of 21 female weaning rats, were given for 6 weeks a basic diet containing 0.025 mg Mo/kg diet as well as 6.3 mg Cu/kg diet, and additionally in their drinking water doses of 0, 5, 10, 50 and 100 mg Mo/L as sodium molybdate (Na2MoO4.2H2O) for 3 weeks until the 21st day of gestation. Six animals in each group were sacrificed after 6 weeks to determine the oestrus cycle length. The remaining 15 animals in each group were mated with untreated males and allowed to continue gestation for 21 days.
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">http://www.who.int/water_sanitation_health/dwq/guidelines/en</a>	No data	01/06/2009	DW	a) 0.07 b) N/A c) N/A	a) mg/L [Note Units] b) N/A	a) 70 b) N/A		a) NOAEL b) N/A c) NOAEL	a) 0.2 b) N/A c) 2	a) mg/L b) N/A c) mg/kg/bw/day	a) 3 b) N/A c) none provided	a) Although an uncertainty factor of 10 would normally be applied to reflect intraspecies variation, it is recognized that molybdenum is an essential element, and a factor of 3 is therefore considered to be adequate (provided in reference) (WHO) b) N/A c) None provided	a) 2 year study of humans exposed via drinking water	a) There are some concerns about the quality of this study. This gives a guideline value of 0.07 mg/litre (rounded figure), which is in the same range as that derived on the basis of the results of toxicological studies in animals and is consistent with the essential daily requirement for molybdenum b) five pairs of Charles River CD mice received 10mg of molybdenum per litre (about 1.5mg/kg/bw/day) in deionised drinking-water for up to 6 months. c) The effects of dietary molybdenum on reproductive ability and pup growth during lactation were studied in Long-Evans rats fed diets containing 0.1, 2, 8, or 14 mg of molybdenum per kg of body weight per day and either 5 or 20 mg of copper per kg for 13 weeks (35).
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	March 2001	01/06/2009	TDI	10	ug/kg/bw/day	10	Medium	TDI oral (based on a NOAEL of 1mg/kg as seen in rats)	10 (TDloral)	ug/kg bw/day		Considered adequate for intrahuman variation (RIVM)		TDI of 10
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	28/10/2003 (based on 1961 study)	01/06/2009	Oral RfD	0.005	mg.kg-1.d-1	5	Medium	LOAEL	0.14	mg.kg-1.d-1	30	Quoted from IRIS. 3 for protection of sensitive human populations and a factor of 10 for the use of a LOAEL, rather than a NOAEL, from a long-term study in a human population. A full factor of 10 is not used for the protection of sensitive human populations because the study was conducted in a relatively large human population (IRIS)	Chronic. Human 6-year to Lifetime dietary exposure study	Koval'skiy, V.V., G.A. Yarovaya and D.M. Shmavonyan. 1961. Changes of purine metabolism in man and animals under conditions of molybdenum biogeochemical provinces. Zh. Obshch. Biol. 22:179-191. (Russian trans.)  Notes to the value quoted: Dose determined from study: molybdenum (Mo) concentration in diet is 10-15 mg/day. Assumed body weight of adult male is 70 kg; 10 mg molybdenum/70-kg body weight = 0.14 mg/kg-day.

## Molybdenum

TDI oral			
Organisation	Target organ/Critical Effect	Reference	Web link
European Food Safety Authority (EFSA)	Reproductive toxicity (oestrus activity, fertility and foetal development). There was no effect on fertility, food and water consumption. Oestrus cycle was prolonged from 1.6 mg/kg bw/day and higher supplementation. Gestational weight, litter size and foetal weights were less than controls for the groups fed 1.6 mg/kg bw/day and higher doses. Histopathology showed delayed histological development of foetal structures, delayed oesophageal development, delayed transfer of foetal haematopoiesis from liver to bone marrow, and delayed myelination of the spinal cord at doses of $\geq 1.6$ mg/kg bw/day. Foetal resorption increased at doses of 1.6 mg/kg bw/day and higher. SO and XDH/XO activity increased with Mo supplementation but less in pregnant animals at dose levels of 1.6 mg/kg bw/day and above.	EFSA 'Tolerable Upper Intake Levels for Vitamins and Minerals' 2006.	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Document/upper_level_opinions_full-part33.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Document/upper_level_opinions_full-part33.pdf?ssbinary=true</a>
WHO Guidelines for drinking water Quality	a) not mentioned b) Excess foetal mortality was observed (-15of238) in F1 generation and 4 (of 242), 5 dead litters and 1 maternal death in F2 generation. The experiment was discontinued after the F3 generation because of the elevated incidence of deaths of offspring, parents and infertility. c) reduced number of litters at the 2 highest Mo concentrations as a result of varying degrees of degeneration and the seminiferous tubules. Lactating mothers at the two highest doses lost less weight during lactation than females in the lower-dose groups, and there were indications that pups from mothers exposed to the highest dose of molybdenum gained less weight at weaning than other pups; these effects were probably due to reductions in milk production associated with high maternal dietary intake of molybdenum.	WHO <a href="http://www.who.int/water_sanitation_health/dwg/chemicals/molybdenum.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/molybdenum.pdf</a>	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/molybdenum.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/molybdenum.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	TDI and TCA provided	Derived by Vermeire et al 1991 as part of the work.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Increased uric acid levels	USEPA IRIS Study by Koval'sky et. al. 1961. IRIS database <a href="http://www.epa.gov/NCEA/iris/subst/0425.htm">http://www.epa.gov/NCEA/iris/subst/0425.htm</a>	<a href="http://www.epa.gov/ncea/iris/subst/0425.htm">http://www.epa.gov/ncea/iris/subst/0425.htm</a>

<b>Molybdenum</b>	<b>CAS Number:</b> 7439-98-7	<b>Assessor A:</b> Nick Struggles, AECOM	<b>Assessor B:</b> Atkins	<b>Final review:</b> Penl/SF
		<b>Date:</b> 01/06/2009	<b>Date:</b> 17/06/2009	<b>Date:</b> 26/08/2009

<b>TDI inhal</b>	<b>Recommended TDInhal</b>	<b>Units</b>	<b>Justification</b>
	3.43	ug.kg-1.d-1	RIVM values chosen. If any of the HSE values were chosen it would be necessary to apply additional Uncertainty Factors which is out with the scope of this work.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	No data	30/06/1905							a) 5 b) 10 c) 10 d) 20	mg/m3			Workplace exposure limit. This list is legally binding, as it reproduces the list of workplace exposure limits (WELs) which have been approved by the Health and Safety Commission	a) Long-term exposure (8-hour TWA limit reference period) - soluble b) Long-term exposure (8-hour TWA limit reference period) - insoluble c) Short-term exposure limit (15minute reference period) - soluble d) Short-term exposure limit (15minute reference period) - insoluble
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	No data	01/06/2009		Human intake of airborne molybdenum is not likely to be a major exposure pathway										
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/03/2001	01/06/2009	TCA		12 ug.m-3	3.43 ( 12 ug.m3 x 20m3/day / 70kg )	Low	NOAEC	100	mg.m-3	1000	Factor of 100 for inter- and intraspecies extrapolation and 10 for semi chronic to chronic exposure	semi chronic	NTP 1997 Study of inhalation of molybdenum trioxide in rats and mice, only effect on body weight was noticed at 300 mg.m-3. After 2 year inhalation exposure of 300 mg.m-3. Concluded changes are similar to other inhalation studies of particulate compounds and not caused by the molybdenum trioxide.

<b>ID oral</b>	<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>
	None		Insufficient data

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type	Description

<b>ID inhal</b>	<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>
	None		Insufficient data

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type	Description

## Molybdenum

TDI inhal			
Organisation	Response	Reference	Web link
Health and Safety Executive (HSE)	not mentioned	EH40/2005 Workplace exposure limits. Table 1: List of approved workplace exposure limits (as consolidated with amendments October 2007)	<a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>
WHO Guidelines for drinking water Quality		Chappell WR. Transport and biological effects of molybdenum in the environment in: WHO 2996 'Molybdenum in Drinking-water Background document for development of WHO Guidelines for Drinking-water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/molybdenum.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/molybdenum.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Inflammatory Lesions	Baars et al. 2001 'Re-evaluation of human-toxicological maximum permissible risk levels' RIVM report 711701 025.	
ID oral			
Organisation	Response	Reference	Web link
ID inhal			
Organisation	Response	Reference	Web link

Molybdenum	CAS 7439-98-7	Assessor A:	Nick Struggles, AECOM	Assessor B:	Atkins	Final review:	Panel/SF
		Date	01/06/2009	Date	17/06/2009	Date	26/08/2009

MDI		Recommended MDI <sub>oral</sub>	Units	Justification: Mean daily intake for adults in food from FSA (1.64 ug/kg.bw/day), equivalent to 114.8µg/day assuming a 70kg adult. WHO notes concentration of Mo in drinking water are typically less than 0.01mg/L (equivalent to 0.02 mg/day for 2L consumed per day). MDI <sub>oral</sub> is sum of contributions from diet and drinking water.			
		134.8	ug day-1				
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Food Standards Agency	01/05/2009	mean dietary exposure for adults	a) estimated 0.123-0.125 b) mean for adults 1.61-1.64 c) toddlers mean 4.8-4.87 d) young people mean 3.01-3.05	a) mg/day b), c), d) ug/kg bw/day	This is slightly higher than the exposure reported in 1994 and 1991 and 1985 (0.11mg/day). These are well within the guidance level for molybdenum of 0.23mg/day as stated in the EVM report and the WHO estimated daily requirement for molybdenum of 0.1-0.3mg/day for adults. The mean dietary exposure for adults was estimated to be 1.61-1.64ug/kg/bw and the high level exposure was 3.03-3.08 ug/kg/bw/day. Estimated intake in toddlers mean (4.8-4.87ug/kg/bw/day) and high level (7.54-8.32ug/kg/bw/day) and for young people mean (3.01-3.05ug/kg/bw/day) and high level (5.77-5.82ug/kg/bw/day).	Page 15. MEASUREMENT OF THE CONCENTRATIONS OF METALS AND OTHER ELEMENTS FROM THE 2006 UK TOTAL DIET STUDY January 2009	<a href="http://www.food.gov.uk/multimedia/pdfs/fsis0109metals.pdf">http://www.food.gov.uk/multimedia/pdfs/fsis0109metals.pdf</a>
Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	01/05/2009	a) and b) food dietary intake c) max recommended level in drinking water d) WHO noted typical drinking water concentration e) Recommended daily requirement of Mo f) drinking water g) supplements h) Estimated maximum intake	a) 0.11mg (mean) b) 0.21mg (97.5%ile) c) 0.07 d) 0.01 e) 0.1-0.3 f) 0.02 g) up to 0.33mg h) 0.21+0.02+0.33=0.56	a) and b) mg c) and d) mg/L e) mg/day for adults f) mg/day g) mg h) mg/day	a) and b) Daily exposure estimates from food Source of data sources, excluding supplements, for men and women (in mg). Mean and 97.5%ile values presented. c) WHO recommended max level of Mo in drinking water d) WHO notes that the concentrations of Mo in drinking water are typically less than 0.01mg/L, however, in areas near mining sites, Mo concentrations up to 0.2mg/L have been reported. e) WHO 1993 estimated daily requirement for molybdenum for adults f) drinking water - (estimated from 0.01mg/L (WHO 1993) g) supplements h) estimated maximum intake (totalled from food (97.5%ile see a), drinking water (see f) and maximum recommended supplements (see g)	a) and b) MAFF 1997. quoted in Safe Upper Limit on Vitamins and Minerals (May 2003) http://cot.food.gov.uk/pdfs/vitmin2003.pdf c), d), e), f), g), h)http://cot.food.gov.uk/pdfs/vitmin2003.pdf	<a href="http://cot.food.gov.uk/pdfs/vitmin2003.pdf">http://cot.food.gov.uk/pdfs/vitmin2003.pdf</a>
European Food Safety Authority (EFSA)	01/05/2009	Estimated dietary exposure (food and drink)	50-400 (mean 128)	ug day-1	Estimated Dietary exposure for Adults in UK.	SCF 1993 study in EFSA 'Tolerable Upper Intake Levels for Vitamins and Minerals' 2006. http://www.efsa.europa.eu/cs/lobServer/Scientific_Document/upper_level_opinions_full-part33.pdf?ssbinary=true	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a>
Scientific Committee on Food (SCF) pre 2002	01/05/2009	mean dietary intake	128	ug/day	Mean dietary intake in the United Kingdom	Previous source: SCF 1993 . Commission of the European Communities. Reports of the Scientific Committee for Food (thirty-first series). Nutrient and energy intakes for the European Community. Opinion Expressed on 11 December 1992. http://ec.europa.eu/food/fs/sc/scf/out89.pdf  Original source: Mills CF, Davis, GK. 1987. Molybdenum. In: Mertz W, ed. Trace Elements in Human and Animal Nutrition. 5th Ed. Vol 1. San Diego: Academic Press, 429-463.	<a href="http://ec.europa.eu/fppd/fs/sc/scf/index_en.html">http://ec.europa.eu/fppd/fs/sc/scf/index_en.html</a>

Molybdenum		CAS 7439-98-7	Assessor A: Date	Nick Struggles, AECOM 01/06/2009	Assessor B: Date	Atkins 17/06/2009	Final review: Date	Panel/SF 26/08/2009
WHO Guidelines for Drinking Water Quality	01/05/2009	Food and Drinking Water	240 for adult men and 100 for women	ug day-1	Estimated total exposures and relative contribution of drinking water - intakes in the USA range from 240ug/day for adult men to 100ug/day for women. In most areas intake via drinking water will not exceed 20ug/day.	Tsongas TA et al. Molybdenum in the diet: an estimate of average daily intake in the United States. American journal of clinical nutrition, 1980, 33:1103-1107 in: <a href="http://www.who.int/water_sanitation_health/dwq/chemicals/molybdenum.pdf">http://www.who.int/water_sanitation_health/dwq/chemicals/molybdenum.pdf</a>	<a href="http://www.who.int/water_sanitation_health/guidelines/en">www.who.int/water_sanitation_health/guidelines/en</a>	
	17/03/2009	Drinking water guideline	0.07	mg/L	Drinking water standard	WHO Drinking Water Guidelines <a href="http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf</a>	<a href="http://www.who.int/water_sanitation_health/guidelines/en">www.who.int/water_sanitation_health/guidelines/en</a>	
	01/05/2009	Drinking Water	10	ug day-1	Levels in drinking water do not usually exceed 10ug/L, however, near mining operations the concentrations in finished water can be as high as 200ug/L. Tap water concentrations as high as 580ug/L have been reported in Colorado.	Molybdenum in Drinking-water. Background document for development of WHO Guidelines for Drinking-water Quality. WHO 2003 Originally published in Guidelines for drinking-water quality, 2nd ed. Vol. 2. Health criteria and other supporting information. World Health Organization, Geneva, 1996.	<a href="http://www.who.int/water_sanitation_health/guidelines/en">www.who.int/water_sanitation_health/guidelines/en</a>	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	01/05/2009	maximal daily intake	4	ug/kg bw/day	Vermeire et al (1991) estimated a maximal daily intake. This estimate has not been refuted by more recent data presented in the report of the US-EPA (1989) and the WHO (1996).	Page 77. RIVM 711701025 Re-evaluation of human-toxicological maximum permissible risk levels, March 2001. <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>	
Health Canada Toxicological Reference Values	01/05/2009	daily dose	2.5-2000 (min-max)	ug/day	for adults >19years. Daily dose.	Page 26. Health Canada. MULTI-VITAMIN/MINERAL SUPPLEMENT MONOGRAPH. October 22, 2007. <a href="http://www.hc-sc.gc.ca/dhp-mpps/alt_formats/hpfb-dgpsa/pdf/prodnatur/multivit_min_mono-eng.pdf">http://www.hc-sc.gc.ca/dhp-mpps/alt_formats/hpfb-dgpsa/pdf/prodnatur/multivit_min_mono-eng.pdf</a>	<a href="http://www.hc-sc.gc.ca/dhp-mpps/alt_formats/hpfb-dgpsa/pdf/prodnatur/multivit_min_mono-eng.pdf">http://www.hc-sc.gc.ca/dhp-mpps/alt_formats/hpfb-dgpsa/pdf/prodnatur/multivit_min_mono-eng.pdf</a>	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	01/05/2009	daily intake	0.075	mg day-1	Based on a site specific report by USEPA for Cady Road. The FDA's adult recommended daily intake for molybdenum is 0.075 mg. By drinking 2 litres of private well water per day, Cady Road residents would consume about 0.040 mg of molybdenum, or a little over half of the daily value.	Appendix F Water Quality and Metals: Molybdenum. Petitioned Health Consultation. ATSDR. <a href="http://www.atsdr.cdc.gov/HAC/pha/cadyroad/cad_p2.html">http://www.atsdr.cdc.gov/HAC/pha/cadyroad/cad_p2.html</a>	<a href="http://www.atsdr.cdc.gov/HAC/pha/cadyroad/cad_p2.html">http://www.atsdr.cdc.gov/HAC/pha/cadyroad/cad_p2.html</a>	
Entrez PubMed	01/05/2009	Dietary Exposure	112	ug day-1	Estimated mean daily intake in the UK	Noel et al (2003) in <a href="http://www.ncbi.nlm.nih.gov/pubmed/12519718?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/12519718?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>	
MDI			Recommended MDIinh 0	Units ug day-1	Justification: WHO study concludes air not a major pathway. Excluded occupational exposure data.			
Organisation	Date	Media	Value	Units	Description	Reference	Web link	
Health Protection Agency	01/05/2009	Air	5	mg.m-3	Occupational exposure limit to Mo compounds soluble (as Mo). Long term exposure limit (8 hr TWA)	EH 40/2005, as consolidated with amendments October 2007 <a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>	<a href="http://www.hpa.org.uk">www.hpa.org.uk</a>	
WHO Guidelines for Drinking Water Quality	01/05/2009	Air	Human intake of airborne molybdenum is not likely to be a major exposure pathway	N/A	Human intake of airborne molybdenum is not likely to be a major exposure pathway	Chappell WR. Transport and biological effects of molybdenum in the environment in: <a href="http://www.who.int/water_sanitation_health/dwq/chemicals/molybdenum.pdf">http://www.who.int/water_sanitation_health/dwq/chemicals/molybdenum.pdf</a>	<a href="http://www.who.int/water_sanitation_health/guidelines/en">www.who.int/water_sanitation_health/guidelines/en</a>	

Substance:		Molybdenum		CAS Number:	7439-98-7 <th>Assessor A:</th> <td>N Struggles, AECOM <th>Assessor B:</th> <td>Atkins <th>Final review:</th> <td>Panel/SF</td> </td></td>	Assessor A:	N Struggles, AECOM <th>Assessor B:</th> <td>Atkins <th>Final review:</th> <td>Panel/SF</td> </td>	Assessor B:	Atkins <th>Final review:</th> <td>Panel/SF</td>	Final review:	Panel/SF																									
Chemical Formula:		Mo		Phase at Ambient Temperature	Solid (Metal) <th>Date:</th> <td>02-Jun-09 <th>Date:</th> <td>17-Jun-09 <th>Date:</th> <td>26-Aug-09</td> </td></td>	Date:	02-Jun-09 <th>Date:</th> <td>17-Jun-09 <th>Date:</th> <td>26-Aug-09</td> </td>	Date:	17-Jun-09 <th>Date:</th> <td>26-Aug-09</td>	Date:	26-Aug-09																									
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H			ADDITIONAL REFERENCES					
							HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCX, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000			INCHEM					
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)			
<b>Required Parameters</b>							mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	8.40E+05	25	Highest value located, for sodium molybdenate	Geomean	Insert Values		Insert Values		Insert Values		0.00E+00		0.00E+00		Insert Values		Insert Values		Insert Values		Insert Values		Insert Values		8.40E+05	8.40E+05	5.00E+01	5.00E+01						
Soil Water Partition Coefficient	cm <sup>3</sup> g <sup>-1</sup>	NA	NA	NA	No data found - though not required for for land uses without plant uptake being modelled by EIC	Average	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a		
Soil-to-plant concentration factor - Green Vegetables	mg kg <sup>-1</sup> FW plant per mg kg <sup>-1</sup> DW soil	NA	n/a	n/a																																
Soil-to-plant concentration factor - Root Vegetables	mg kg <sup>-1</sup> FW plant per mg kg <sup>-1</sup> DW soil	NA	n/a	n/a																																
Soil-to-plant concentration factor - Tuber Vegetables	mg kg <sup>-1</sup> FW plant per mg kg <sup>-1</sup> DW soil	NA	n/a	n/a																																
Soil-to-plant concentration factor - Herbaceous Fruit	mg kg <sup>-1</sup> FW plant per mg kg <sup>-1</sup> DW soil	NA	n/a	n/a																																
Soil-to-plant concentration factor - Shrub Fruit	mg kg <sup>-1</sup> FW plant per mg kg <sup>-1</sup> DW soil	NA	n/a	n/a																																
Soil-to-plant concentration factor -	mg kg <sup>-1</sup> FW plant per mg kg <sup>-1</sup> DW soil	NA	n/a	n/a																																
Soil-Plant availability correction factor	Dimensionless	NA	n/a	n/a																																
Root-shoot, root-root store, root-tuber and root to fruit correction factors	Dimensionless	NA	n/a	n/a																																
Dermal Absorption factor	Dimensionless	NA	0	n/a	Source: SR3 for metals in absence of other data																															
Soil to dust transport factor	Dimensionless	NA	0.5	n/a	Source: SR3 in absence of other data																															

1,1,2 trichloroethane	CAS Number: 79-00-5	Assessor A: J Thornton, Golder Associates	Assessor B: M Evans, Firth Consultants	Final review: Panel/SF
		Date: 15/04/2009	Date: 29/04/2009	Date: 25/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	No	Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen - TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	4	ug.kg-1.d-1	USEPA IRIS and RIVM (chronic) value used. It is noted that the USEPA PPRTV is more recent, although it is a sub-chronic RfD and provisional.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>		15/04/2009	Classified Class 3: TDI									
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	1996	15/04/2009	Maximum permissible risk level (MPR) same as TDI		4 ug.kg-1.d-1	4	Provisional value - MUCH UNCERTAINTY	NOAEL	3.9	mg.kg-1.day-1	1000	10 x interspecies, 10 x intraspecies, 10 subchronic not chronic study
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	Unknown	15/04/2009	No Health based criteria, Not a priority contaminant									
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Dec-89	15/04/2009	Minimal Risk Level acute exposure		0.3 mg.kg-1.day-1	300	Final	Unknown	Unknown	Unknown	100	Unknown
		Dec-89	15/04/2009	Minimal Risk Level intermediate exposure		0.04 mg.kg-1.day-1	40	Final	Unknown	Unknown	Unknown	100	Unknown
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	Feb-95	15/04/2009	RfD		0.004 mg.kg-1.day-1	4	Medium	NOAEL	3.9	mg.kg-1.day-1	1000	10 x interspecies, 10 x intraspecies, 10 subchronic not chronic study
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	17-10-2006	29-07-2009	p-sRfD (provisional sub-chronic reference dose)		0.0039 mg.kg-1.day-1	3.9	Low	NOAEL	3.9	mg/kg-day	1000	10 for extrapolation from mice to humans, 10 for protection of sensitive individuals, and 10 for deficiencies in the database
USEPA Region 9 PRGs	<a href="http://www.epa.gov/region09/superfund/prg/index.html">http://www.epa.gov/region09/superfund/prg/index.html</a>	Apr-09	26/05/2009	RfDo	0.004	mg.kg-1.day-1	4	No data	No data	No data	No data	No data	No data
RAIS	<a href="http://rais.ornl.gov/homepage/rap_tool.shtml">http://rais.ornl.gov/homepage/rap_tool.shtml</a>	1985	26/05/2009	RfDo	0.004	mg.kg-1.day-1	4	Medium	NOAEL/LOAEL	No data	No data	1000	No data
Adaptive Risk Assessment Modelling System (ARAMS™)	<a href="http://el.erdc.usace.army.mil/arams/">http://el.erdc.usace.army.mil/arams/</a>	Links to IRIS and RAIS	26/05/2009	No data	No data	No data	No data	No data	No data	No data	No data	No data	No data
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rr.htm">http://www.tceq.state.tx.us/remediation/rr.htm</a>	No data	26/05/2009	RfDo	0.004	mg.kg-1.day-1	4	No data	No data	No data	No data	No data	No data

TDI inhal	Recommended TDlinhal	Units	Justification
	4.85	ug.kg-1.d-1	Only data available (RIVM)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>		15/04/2009	Classified Class 3: TDI									
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	March 1998	15/04/2009	Maximum permissible risk level (MPR) same as TDI		17 ug.m-3	4.857142857	Provisional value - MUCH UNCERTAINTY	NOAEL	82	mg/m3	1000	10 x interspecies, 10 x intraspecies, 10 subchronic not chronic study

## 1,1,2 trichloroethane

## TDI oral

Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
International Agency for Research on Cancer (IARC)					
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	Mice subchronic	90 day drinking water study in mice	CNS, liver, kidneys	Janssen et al. 1998 based on US EPA IRIS (1995). Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701004.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701004.pdf</a>
Health Canada Toxicological Values					
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Unknown	Unknown	Neurological end point	ATSDR MRL for Hazardous Substances, last updated Dec 2008	<a href="http://www.atsdr.cdc.gov/mrls/index.html#bookmark02">http://www.atsdr.cdc.gov/mrls/index.html#bookmark02</a>
	Unknown	Unknown	Hepatic end point	ATSDR MRL for Hazardous Substances, last updated Dec 2008	<a href="http://www.atsdr.cdc.gov/mrls/index.html#bookmark02">http://www.atsdr.cdc.gov/mrls/index.html#bookmark02</a>
USEPA Integrated Risk Information System (IRIS)	Mouse Subchronic Drinking Water Study	Mice exposed via drinking water for 90 days, various doses.	Liver	US EPA IRIS: Sanders, V.M., K.L. White, Jr., G.M. Shopp, Jr. and A.E. Munson. 1985. Humoral and cell-mediated immune status of mice exposed to 1,1,2-trichloroethane. Drug Chem. Toxicol. 8(5): 357-372. and White, K.L., Jr., V.M. Sanders, V.W. Barnes, G.M. Shopp, Jr. and A.E. Munson. 1985. Toxicology of 1,1,2-trichloroethane in the mouse. Drug Chem. Toxicol. 8(5): 333-355.	<a href="http://www.epa.gov/ncea/iris/subst/0198.htm#studoral">http://www.epa.gov/ncea/iris/subst/0198.htm#studoral</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Subchronic mouse study	Groups of male and female CD-1 mice (16/sex/group) were exposed to 1,1,2-trichloroethane in the drinking water for 90 days at concentrations of 20, 200, or 2000 mg/L, which the researchers estimated to provide doses of 0, 4.4, 46, and 305 mg/kg-day for males and 0, 3.9, 44, and 384 mg/kg-day for females (White et al., 1985; Sanders et al., 1985).	Liver	Sanders, V.M., K.L. White Jr., G.M. Shopp et al. 1985. Humoral and cell-mediated immune status of mice exposed to 1,1,2-trichloroethane. Drug Chem. Tox. 8: 357-372. AND White, K.L. Jr., V.M. Sanders, D.W. Barnes et al. 1985. Toxicology of 1,1,2-trichloroethane in the mouse. Drug Chem. Tox. 8: 333-355.	Not available online. Document reference: US EPA (2006). Provisional Peer Reviewed Toxicity Values for 1,1,2-Trichloroethane (CASRN 79-00-5), Derivation of a Subchronic Oral RfD, Superfund Health Risk Technical Support Center, National Center for Environmental Assessment, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH 45268.
USEPA Region 9 PRGs	No data	No data	No data	No data	<a href="http://www.epa.gov/region09/superfund/prg/pdf/master_sl_table_bwrun_APRIL2009.pdf">http://www.epa.gov/region09/superfund/prg/pdf/master_sl_table_bwrun_APRIL2009.pdf</a>
RAIS	No data	Mouse	Clinical serum chemistry	White et al. (1985)	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select">http://rais.ornl.gov/cgi-bin/tox/TOX_select</a>
Adaptive Risk Assessment Modelling System (ARAMS™)	No data	No data	No data	No data	No data
Texas Commission on Environmental Quality	No data	No data	No data	No data	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppls.html</a>

## TDI inhal

Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)					
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Multiple species, subchronic	6 month study on several species	CNS, liver, kidneys	Janssen et al. 1998 based on Dow (1981). Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701004.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701004.pdf</a>

1,1,2 trichloroethane	CAS Number:	79-00-5	Assessor A:	J Thornton, Golder Associates	Assessor B:	M Evans, Firth Consultants	Final review:	Panel/SF
			Date	15/04/2009	Date	29/04/2009	Date	25/08/2009

ID oral	Recommended IDoral	Units	Justification
	n/a		Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
European Chemicals Bureau (ECB)	<a href="http://ecb.irc.it/">http://ecb.irc.it/</a>		15/04/2009	Carcinogenic Category 3						
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	Verification Date — 07/23/1986	15-Apr-09	C - Possible human carcinogen	Hepatocellular carcinomas and pheochromocytomas in one strain of mice forms the basis for this classification. Carcinogenicity was not shown in rats. 1,1,2 Trichloroethane is structurally related to 1,2-dichloroethane, a probable human carcinogen	Oral slope factor	5.70E-02	(mg.kg-1.d-1)-1	Dose-related increases in hepatocellular carcinomas were observed in adequate numbers or mice of both sexes. Background incidence of this tumour type is generally high. Modelling was done on only one data set.	Extrapolation Method — Linearized multistage procedure, extra risk

ID inhal	Recommended IDinhal	Units	Justification
	n/a		Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	Verification Date — 07/23/1986	15-Apr-09			Inhalation unit risk	1.60E-05	(µg.m-3)-1	Dose-related increases in hepatocellular carcinomas were observed in adequate numbers or mice of both sexes. Background incidence of this tumour type is generally high. Modelling was done on only one data set.	Extrapolation Method — Linearized multistage procedure, extra risk

## 1,1,2 trichloroethane

ID oral					
Organisation	Study type	Description	Response	Reference	Web link
European Chemicals Bureau (ECB)				Meeting of the Commission Working Group on the Classification and Labelling of Dangerous Substances, ECB Ispra, 16-18 January 2002. ECBI/15/02 Rev 3.	<a href="http://ecb.jrc.ec.europa.eu/documents/Classification-Labelling/ADOPTED_SUMMARY_RECORDS/1502r3_sr_CM0102.pdf">http://ecb.jrc.ec.europa.eu/documents/Classification-Labelling/ADOPTED_SUMMARY_RECORDS/1502r3_sr_CM0102.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels				Kreule P, Swartjes FA (1998) Proposals for Intervention Values for soil and groundwater, including the calculation of the human-toxicological serious soil contamination concentrations: Fourth series of compounds. RIVM rapport 711701005.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701005.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701005.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Oral, gavage	Technical grade (92.7%) 1,1,2- trichloroethane administered by gavage in corn oil to Osborne-Mendel rats and B6C3F1 mice. 4 groups of 50 (2 sexes x 2 species) given an average of 139 mg.kg-1.d-1 1,1,2-TCA. 4 groups of 50 (2 sexes x 2 species) given an average of 279 mg.kg-1.d-1 1,1,2-TCA. 4 groups of 20 (2 sexes x 2 species) were used as control. By two statistical tests, treatment of mice was found to be associated with increased incidence of hepatocellular carcinomas. Tumours were found in treated rats that were not found in controls but there was no statistically significant increase in tumour incidence in rats as a function of treatment	Hepatocellular carcinoma	NCI (National Cancer Institute). 1978. Bioassay of 1,1,2-trichloroethane for possible carcinogenicity. U.S. DHEW Tech. Rep. Ser. 74. Publ. No. NIH 78-1324.	<a href="http://www.epa.gov/ncea/iris/subst/0198.htm#quaoral">http://www.epa.gov/ncea/iris/subst/0198.htm#quaoral</a>
ID inhal					
Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)		This inhalation risk estimate was calculated from the oral exposure data described in the ID oral section above			<a href="http://www.epa.gov/ncea/iris/subst/0198.htm#quaoral">http://www.epa.gov/ncea/iris/subst/0198.htm#quaoral</a>

<b>1,1,2 trichloroethane</b>	CAS 79-00-5	Assessor A:	Jeff Thorton (Golder Assoc.)	Assessor B:	Melinda Evans (Firth Consultants)	Final review:	Panel/SF
		Date	15/04/2009	Date	29/04/2009	Date	25/08/2009
<b>MDI</b>			<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	Justification: Value of 0.24 µg.day <sup>-1</sup> selected from European study (RIVM). OECD Report is based on a 'worst case' scenario using Japanese data. The 1,1,1-TCA isomer has a TOX report with an oral MDI of 0.2 µg/day which is comparable.		
			<b>0.24</b>	<b>ug day<sup>-1</sup></b>			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS INCHEM	15/04/2009	Drinking water	2.60E+00	ug.day-1	Based on the highest PEC of 1.30 x 10 <sup>-3</sup> mg/l (1.3 ug.L) ASSUMING 2 L/day for an adult	OECD SIDS 1,1,2-trichloroethane SIDS Initial Assessment Report, March 2000, section 4.1.3 ( <a href="http://www.inchem.org/documents/sids/sids/79005.pdf">http://www.inchem.org/documents/sids/sids/79005.pdf</a> )	<a href="http://inchem.org/">http://inchem.org/</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Food and drink	0.24	ug day-1	Study from Germany 1980-1983	Janssen et al. 1998. Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998. Page 79.	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Drinking water	no data	-	US	Toxicological Profile for 1,1,2-Trichloroethane. December 1989. <a href="http://www.atsdr.cdc.gov/toxprofiles/tp148-c5.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp148-c5.pdf</a>	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
Other	06/04/2009	Food and drinking water	Rarely encountered	-	US	Technology Transfer Network Air Toxics Web Site. Hazard Summary-Created in April 1992; Revised in January 2000	<a href="http://epa.gov/ttn/air/hlthef/tri-etha.html">http://epa.gov/ttn/air/hlthef/tri-etha.html</a>
	06/04/2009	Drinking water	0.24	µg.kg-1.day-1	Japan: expected quantities of the maximum oral exposure. Suspect units quoted are incorrect should be ug.day-1.	Japanese Chemical Substances Control Document: 1,1,2-trichloroethane	<a href="http://www.env.go.jp/en/chemi/chemicals/profile_erac/profile5/pf1-18.pdf">http://www.env.go.jp/en/chemi/chemicals/profile_erac/profile5/pf1-18.pdf</a>

<b>1,1,2 trichloroethane</b>	CAS 79-00-5	Assessor A:	Jeff Thorton (Golder Assoc.)	Assessor B:	Melinda Evans (Firth Consultants)	Final review:	Panel/SF
		Date	15/04/2009	Date	29/04/2009	Date	25/08/2009
<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	Justification: European study (RIVM) and Howard et al quote a value of 1 ug/ day. The higher range of 1.1 to 5.5 ug/day is based on old US data.		
			<b>1</b>	<b>ug day-1</b>			
<b>Organisation</b>		<b>Media</b>	<b>Value</b>	<b>Units</b>	<b>Description</b>	<b>Reference</b>	<b>Web link</b>
<b>Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels</b>	15-Apr-09	Air	1	ug day-1	Air study in Germany 1986-1987, assuming adult inhales 20 m <sup>3</sup> /day (0.05 m <sup>3</sup> )	Janssen et al. 1998. Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998, Page 79	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
<b>US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels</b>	15-Apr-09	Air	1.1-5.5	ug.day-1	Average daily intake for 'background' exposure in US	Toxicological Profile for 1,1,2-Trichloroethane. December 1989. <a href="http://www.atsdr.cdc.gov/toxprofiles/tp148-c5.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp148-c5.pdf</a> , page 71	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
<b>Other</b>	15-Apr-09	Ambient air	1	ug/day	US study of 930 samples with a median concentration of 9.1 parts per trillion	Howard et al 1990, Handbook of Env Fate and Exposure data for Organic chemicals , Volume 2	
	06/04/2009	Ambient air	0.01-0.05	ppb	US	Technology Transfer Network Air Toxics Web Site. Hazard Summary-Created in April 1992; Revised in January 2000. Based on ATSDR report	<a href="http://epa.gov/ttn/atw/hlthef/tri-etha.html">http://epa.gov/ttn/atw/hlthef/tri-etha.html</a>
	06/04/2009	Outdoor residential air	All below detection limit	Detection Limit unknown	Personal exposures among 50 persons and microenvironment concentrations of PM <sub>2.5</sub> , VOC, NO <sub>2</sub> and CO in Oxford, UK in 1998-2000	Lai et al., Atmospheric Environment 38 (2004), 6399-6410	<a href="http://www.ktl.fi/expoplatform/concddb/ui/index.php?Option=object&amp;Object=683">http://www.ktl.fi/expoplatform/concddb/ui/index.php?Option=object&amp;Object=683</a>
	06/04/2009	Outdoor air	0.02	ug.m-3	Predicted maximum exposure concentration for inhalation exposure to human beings	Japanese Chemical Substances Control Document: 1,1,2-trichloroethane	<a href="http://www.env.go.jp/en/chemi/chemicals/profile_erac/profile5/pf1-18.pdf">http://www.env.go.jp/en/chemi/chemicals/profile_erac/profile5/pf1-18.pdf</a>

Substance:	1,1,2 Trichloroethane	CAS Number:	79-00-5	Assessor A:	M Evans, Firth Consultants	Assessor B:	Jeff Thornton, Golders	Final review:	Panel/SF
Chemical Formula:	C2H3Cl3	Phase at Ambient Temperature:	Liquid	Date:	31-Mar-09	Date:	06-May-09	Date:	25-Aug-09

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oe.cd.org/scripts/hpw/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000						
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	
<b>Required Parameters</b>																																		
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	133.4033	n/a	Median value of consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)				
							Average	133.42	133.42	n/a	133.404	133.404	n/a	133.49	133.49	n/a	133.4	133.4	n/a	133.4	133.4	n/a	133.4	133.4	n/a	133.4033	133.4033	n/a	133.4	133.4	n/a			
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	9.20E+01	25	No consistent range most recent review chosen (Lide 2008)		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)				
							Geomean	1.20E-03	1.22E+02	20	9.20E-02	9.20E+01	25	9.21E+01	92.1	25	8.79E+01	25	8.79E+01	25	8.79E+01	25	no data	#VALUE!	25	1.10E+00	9.12E+01	25	no data	#VALUE!	25			
								1.20E-03	1.22E+02	20	9.20E-02	9.20E+01	25	92.1	92.1	25	92.1	25	92.1	25	92.1	25	no data	#VALUE!	25	9.12E+01	9.12E+01	25	no data	#VALUE!	25			
								94.2	94.2	20	94.2	94.2	25	94.2	94.2	25	94.2	25	94.2	25	94.2	25	no data	#VALUE!	25	7.72E+01	7.72E+01	25	no data	#VALUE!	25			
								78.4	78.4	20	78.4	78.4	25	78.4	78.4	25	78.4	25	78.4	25	78.4	25	no data	#VALUE!	25	7.72E+01	7.72E+01	25	no data	#VALUE!	25			
								81.4	81.4	20	81.4	81.4	25	81.4	81.4	25	81.4	25	81.4	25	81.4	25	no data	#VALUE!	25	8.36E+01	8.36E+01	25	no data	#VALUE!	25			
								74.94	74.94	20	74.94	74.94	25	74.94	74.94	25	74.94	25	74.94	25	74.94	25	no data	#VALUE!	25	8.36E+01	8.36E+01	25	no data	#VALUE!	25			
								97.34	97.34	20	97.34	97.34	25	97.34	97.34	25	97.34	25	97.34	25	97.34	25	no data	#VALUE!	25	8.36E+01	8.36E+01	25	no data	#VALUE!	25			
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	4.49E+03	10	Median value @ 10C chosen as consistent range		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	
							Geomean	4.42E+03	4.42E+03	20	4.59E+00	4590	25	4.47E+03	10	10	#VALUE!	#VALUE!	10	4.66E+03	4.66E+03	10	4.33E+03	4.33E+03	10	4.49E+03	4.49E+03	10	4.33E+03	4.33E+03	10			
								4.42E+03	4.42E+03	20	4.59E+00	4590	25	4.47E+03	10	10	#VALUE!	#VALUE!	10	4.66E+03	4.66E+03	10	4.33E+03	4.33E+03	10	4.49E+03	4.49E+03	10	4.33E+03	4.33E+03	10			
								4580	4.58E+03	20	4400	4.40E+03	25	4380	4.38E+03	10	4394	4.39E+03	10	4590	4.59E+03	10	no data	#VALUE!	10	4659	4.66E+03	10	no data	#VALUE!	10			
Chemical Boiling Point (ambient pressure)	K	n/a	3.87E+02	n/a	Median value of consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	
							Average	113.8	386.95	n/a	113.8	386.95	n/a	113.8	386.95	n/a	113.5	386.65	n/a	113.8	386.95	n/a	112.5	385.65	n/a	386.8	386.80	n/a	114	387.15	n/a	114	387.15	n/a
Chemical Melting Point (ambient pressure)	K	n/a	2.37E+02	n/a	Median value of consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	
							Average	-36.5	236.65	n/a	-36.3	236.85	n/a	-36.3	236.85	n/a	-35	238.15	n/a	-36.5	236.65	n/a	-37	236.15	n/a	no data	no data	n/a	no data	no data	n/a	-36	237.15	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	2.38	n/a	No consistent range - most recent review chosen (Lide 2008)		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	
							Average	2.07	2.07	n/a	2.38	2.38	n/a	2.17	2.17	n/a	no data	no data	n/a	1.98	1.98	n/a	no data	no data	n/a	no data	no data	n/a	2.35	2.35	n/a	2.35	2.35	n/a
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	1.15E+02	n/a	single literature value		cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	
							Average	n/a	n/a	n/a	n/a	n/a	n/a	114.5	114.50	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	34140.4943	3.41E+04	Normal Boiling Point	Calculated value chosen - this is similar to range of reported values		KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	
							Average	n/a	n/a	n/a	34.82	34820	Normal Boiling Point	37.07	37070	Normal Boiling Point	34.23	34230	Normal Boiling Point	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	34.82	34820	Normal Boiling Point	n/a	n/a	n/a
Chemical Critical Point temperature (ambient pressure)	K	601.6846236	602	n/a	Calculated value chosen - this is consistent to range of reported values		K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	
							Average	n/a	n/a	n/a	602	602.00	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	602	602.00	n/a	no data	#VALUE!	n/a	n/a
Critical Pressure	atm	44.21472579	44.2	?	Calculated value chosen - this is consistent to range of reported values		Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	
							Average	n/a	n/a	n/a	44.8	44.21416235	?	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	no data	#VALUE!	n/a	n/a	n/a	n/a	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	1.75E-02	10	Estimated from parameters above using Clayton relationship or direct calculation
Vapour pressure at ambient soil temperature	Pa	1386	10	Estimated from parameters above using Grain-Watson method
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	7.58E-06	10	Estimated from parameters above using Wilkie-Lee method
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	5.99E-10	10	Estimated from parameters above using Hayduk and Laudie method
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	2.03	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

<b>1, 1-Dichloroethane</b>	<b>CAS Number:</b>	<b>75-34-3</b>	Assessor A: J Thornton, Golder Associates	Assessor B: N Dixon, Worley Parsons	Final review: Panel/SF	
	Date	15/04/2009	Date	06/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Y	Y	Y	-	Insufficient evaluation to determine with respect to a human carcinogen - TDloral applied to oral, dermal and inhalation routes
Apply IDoral to exposure routes?	-	-	-		
Apply TDlinh to exposure routes?	N	N	N		Insufficient data available to with sufficient details to derive inhalation HCV
Apply IDinh to exposure routes?	-	-	-		

TDI oral	Recommended TDloral	Units	Justification
	200	ug.kg-1.d-1	PPRTV value as only data with sufficient details to derive HCV

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/authorized.shtml">http://rais.ornl.gov/tox/authorized.shtml</a>	27/09/2006	28/07/2009	Chronic oral reference dose	0.2	mg.kg day-1	200	Low	NOAEL	1000 mg.kg day-1 administered 5 days/week adjusted to 714.3 mg.kg day-1 for continuous exposure	mg.kg day-1
USEPA-Regional Screening Level (RSL)	<a href="http://www.epa.gov/region09/superfund/prg/index.html">http://www.epa.gov/region09/superfund/prg/index.html</a>	01/04/2009	05/06/2009	Reference dose	0.2	mg.kg day-1	200	Unknown	Unknown	Unknown	Unknown
Risk Assessment Information System	<a href="http://rais.ornl.gov/homepage/rap_tool.shtml">http://rais.ornl.gov/homepage/rap_tool.shtml</a>	13/02/1998	05/06/2009	Chronic oral reference dose	0.1	mg.kg day-1	100	Unknown	NOAEL	115	mg.kg day-1
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.htm">http://www.tceq.state.tx.us/remediation/rrr.htm</a>	01/03/2006	05/06/2009	Oral reference dose	0.1	mg.kg day-1	100	Unknown	Unknown	Unknown	Unknown

**1, 1-Dichloroethane**

TDI oral
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Organisation	UF	UF description	Study type	Description	Target organ/Critical Effect	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	3000	10 for extrapolation from a sub chronic study, 10 interspecies extrapolation, 10 human variability and 3 for database deficiencies	Subchronic study on male Sprague-Dawley rats. The rats were treated with 1,1-dichloroethane doses of 0, 500, 1000, 2000, or 4000 mg/kg-day by gavage in corn oil, 5 days/week for 13 weeks. Body weights were recorded weekly. Urine was collected every two weeks from half of the animals in each dose group for measurement of protein, glucose, and selected enzyme markers of toxicity (acid phosphatase, N-acetylglucosaminidase, alkaline phosphatase, and maltase). Blood was collected from the remaining half of the animals in weeks 0, 4, 8, and 12 for measurement of serum enzyme markers of toxicity (alanine aminotransferase, sorbitol dehydrogenase, ornithine-carbonyl transferase, and blood urea nitrogen). At study termination, the liver and kidney were weighed and assayed for nonprotein sulfhydryl content, and samples from these organs and the lung, brain, adrenal, stomach, spleen, testes, and epididymis were collected for histological examination.	Based on the transitory and reversible increase in urinary enzymes (ACP) indicative of renal injury at 8 weeks, the 1000 mg/kg-day dose was chosen to be a NOAEL and the 2000 mg/kg-day dose as LOAEL	Kidneys	Muralidhara, S., R. Ramanathan, S.M. Mehta et al. 2001. Acute, subacute, and subchronic oral toxicity of 1,1-dichloroethane in rats: application to risk evaluation. Toxicol. Sci. 64: 134-145.	-
USEPA-Regional Screening Level (RSL)	Unknown	Unknown	Unknown	Unknown	Unknown	EPA's Provisional Peer Reviewed Toxicity Values (PPRTVs)	<a href="http://www.epa.gov/region09/superfund/prg/pdf/ressoil_sl_table_run_APRIL2009.pdf">http://www.epa.gov/region09/superfund/prg/pdf/ressoil_sl_table_run_APRIL2009.pdf</a>
Risk Assessment Information System	1000	Not given	Based on a 13-week inhalation study in rats and route-to-route extrapolation	Unknown	Unknown	Tox study by Hofmann et al., 1971 and reference from HEAST (EPA 1993)	<a href="http://rais.ornl.gov/tox/profiles/1_1_dichloroethane_f_V1.shtml">http://rais.ornl.gov/tox/profiles/1_1_dichloroethane_f_V1.shtml</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtox_chph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtox_chph_2006.xls</a>

<b>1, 1-Dichloroethane</b>	<b>CAS Number:</b>	<b>75-34-3</b>	Assessor A: J Thornton, Golder Associates	Assessor B: N Dixon, Worley Parsons	Final review: Panel/SF	
	Date	15/04/2009	Date	06/05/2009	Date	28/08/2009

<b>TDI inhal</b>	<b>Recommended TDIinhal</b>	<b>Units</b>	<b>Justification</b>
	-	ug.kg-1.d-1	Insufficient data with sufficient details to derive HCV

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	01/10/2007	16/04/2009	Workplace exposure limit	100	ppm	-	Unknown	Unknown	100	ppm
Risk Assessment Information System	<a href="http://rais.ornl.gov/homepage/rap_tool.shtml">http://rais.ornl.gov/homepage/rap_tool.shtml</a>	13/02/1998	05/06/2009	Chronic inhalation reference dose	0.5	mg.m-3	-	Unknown	NOAEL	138	mg.kg day-1
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.htm">http://www.tceq.state.tx.us/remediation/rrr.htm</a>	01/03/2006	05/06/2009	Oral reference dose	0.11	mg.kg day-1	-	Unknown	Unknown	Unknown	Unknown

**1, 1-Dichloroethane**

TDI inhal

Organisation	UF	UF description	Study type	Description	Response	Reference	Web link
Health and Safety Executive (HSE)	Unknown	Unknown	Unknown	Work place exposure limit	Unknown	Table 1. List of approved workplace exposure limits (as consolidated with amendments October 2007) EH40/2005 Workplace exposure limits.	<a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>
Risk Assessment Information System	1000	Not given	Based on an inhalation study on cats: critical effect--kidney damage	Unknown	Unknown	Tox study by Hofmann et al., 1971 and reference from HEAST (EPA 1993)	<a href="http://rais.ornl.gov/tox/profiles/1_1_dichloroethane_f_V1.shtml">http://rais.ornl.gov/tox/profiles/1_1_dichloroethane_f_V1.shtml</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtox/chph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtox/chph_2006.xls</a>

1,1-dichloroethane	CAS 75-34-3	Assessor A: J Thornton, Golder Associates	Assessor B: N Dixon, WorleyParsons	Final review: Panel/SF
		Date: 16/04/2009	Date: 06/05/2009	Date: 28/08/2009

MDI			Recommended MDI <sub>oral</sub>	Units	Justification: ata from WHO, only data from SR2 listed sources
			20	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Pesticides Safety Directorate	01/04/2009					No data	<a href="http://www.pesticides.gov.uk">www.pesticides.gov.uk</a>
Committee on Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	01/04/2009					No data	<a href="http://www.advisorybodies.doh.gov.uk/coc/index.htm">www.advisorybodies.doh.gov.uk/coc/index.htm</a>
Committee on Mutagenicity of Chemicals in Food, Consumer Products and the Environment (COM)	01/04/2009					No data	<a href="http://www.advisorybodies.doh.gov.uk/com/">www.advisorybodies.doh.gov.uk/com/</a>
WHO Guidelines for Drinking Water Quality	14/04/2009	Drinking Water	20	ug/day	Report on DCA (2003) using data presented, this assumes intake of drinking water at 10ug/day (US data) and 2 L per day	<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/1,1-Dichloroethane.pdf">http://www.who.int/water_sanitation_health/dwa/guidelines/1,1-Dichloroethane.pdf</a>	<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/en">www.who.int/water_sanitation_health/dwa/guidelines/en</a>
Howard et al	15/04/2009	Drinking water	0 - 1.2	ug/day	Data presented in Howard et al, 1990. States that exposure via food is probably insignificant.	Howard et al 1990, Handbook of Env Fate and Exposure data for Organic chemicals , Volume 2, p 146	

MDI			Recommended MDI <sub>inh</sub>	Units	Justification: Two sources quote a value of 4 ug.day <sup>-1</sup> (both WHO). US study cites a range of 1.0 to 5.4 ug.day <sup>-1</sup> (ECB)
			4	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
European Chemicals Bureau (ECB)	14/04/2009	ambient air	1-5.4	ug.day <sup>-1</sup>	0.05-0.27 ug.m <sup>3</sup> from USA data	IUCLD dataset	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>
WHO Guidelines for Drinking Water Quality	06/04/2009	ambient air	4.4	ug.day <sup>-1</sup>	Median value of 0.22 ug/m <sup>3</sup> from study in USA		<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/en">www.who.int/water_sanitation_health/dwa/guidelines/en</a>
WHO Air Quality Guidelines for Europe	14/04/2009	ambient air	4	ug.day <sup>-1</sup>	Report on DCA (2003), exposure is greatest through ambient air. Median value.	<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/1,1-Dichloroethane.pdf">http://www.who.int/water_sanitation_health/dwa/guidelines/1,1-Dichloroethane.pdf</a>	<a href="http://www.euro.who.int/activities/20050222_2">www.euro.who.int/activities/20050222_2</a>
Toxicological Data Network (TOXNET)	06/04/2009	Ambient air	4.94	ug.day <sup>-1</sup>	Medium value of 0.061 ppb recorded in 455 US samples from urban and suburban air. Converted to 4.94 ug.day <sup>-1</sup> (0.0409*0.061*MW)	Brodzinsky R, Singh HB; Volatile Organic Chem in the Atmos, An Assess of Available Data; Menlo Park, CA: Atmos Sci Cent, SRI Internatl 68-02-3452 pp. 198 (1982)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
Other	15/04/2009	Ambient air	5	ug.day <sup>-1</sup>	Data presented in Howard et al, 1990 assuming background of 61 ppt	Howard et al 1990, Handbook of Env Fate and Exposure data for Organic chemicals , Volume 2, p 146	

Substance:	1,1-dichloroethane	CAS Number:	75-34-3	Assessor A	J Thornton, Golder Associates	Assessor B	N Dixon, Worley Parsons	Final Review	Panel/SF
Chemical Formula:	C2H4Cl2	Phase at Ambient Temperature	Liquid	Date:	16-Apr-09	Date:	06-May-09	Date:	28/08/2009

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H														
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)									
<b>Required Parameters</b>																																										
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	98.96	n/a	5 identical values in consistent range.	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)									
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	5.95E+02	25	2 values the same from a consistent range.	Geomean	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)									
						5.87E-03	5.95E+02	25	6.30E-01	6.30E+02	25	5.84E+02	584	25	5.84E+02	584	n/a	n/a	n/a	5.45E-03	552.22125	25	no data	#VALUE!	25	5.90E+02	590	25	no data	#VALUE!	25	5.90E+02	590	25	no data	#VALUE!	25					
													436	436																												
													714.9	714.9																												
													569	569																												
													594.9	594.9																												
													561	561																												
													438.8	438.8																												
													594.6	594.6																												
													552	552																												
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	3.666E+03	10	Only 2 sources had 10 degrees C data. NIST data was selected since it is based on several studies and is reasonable based on the other data at 20 and 25 degrees C.	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)									
						5.06E+03	5.06E+03	25	5.00E+00	5000	25	5.00E+03	5000	20	#VALUE!	#VALUE!	5.59E+03	5.59E+03	10	no data	#VALUE!	7.44E+03	7.44E+03	10	no data	#VALUE!	7.44E+03	7.44E+03	10	no data	#VALUE!	7.44E+03	7.44E+03	10								
Chemical Boiling Point (ambient pressure)	K	n/a	3.3045E+02	n/a	4 values the same in consistent range.	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)									
						57.3	330.45	n/a	57.3	330.45	n/a	57.3	330.45	n/a	57.3	330.45	n/a	57.3	330.45	n/a	57.3	330.45	n/a	no data	#VALUE!	n/a	330.5	330.50	n/a	no data	#VALUE!	n/a	330.5	330.50	n/a	no data	#VALUE!	n/a				
Chemical Melting Point (ambient pressure)	K	n/a	1.7600E+02	n/a	3 values the same (to 3 sig. figures) in consistent range.	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)									
						-96.98	176.17	n/a	-96.9	176.25	n/a	-96.7	176.45	n/a	-98	175.15	n/a	-97.4	175.75	n/a	no data	#VALUE!	n/a	174.00	174.00	n/a	176.70	176.70	n/a	176.50	176.50	n/a	no data	#VALUE!	n/a							
Log Octanol - Water Coefficient	Dimensionless	n/a	1.79E+00	n/a	3 values the same across consistent range.	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)									
						1.79	1.79	n/a	1.79	1.79	n/a	1.79	1.79	n/a	1.82	1.82	n/a	1.79	1.79	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a							
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	9.360E+01	n/a	Single source	Average	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a										
						93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a	93.6	93.60	n/a							
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	28872.37561	2.9610E+04	Normal Chemical Boiling Point	Median value of 3 from a consistent range.	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a										
						28.85	28850	n/a	28.85	28850	n/a	30.62	30620	n/a	28.6	28600	n/a	30.77	30770	n/a	30.83	30830	n/a	30.62	30620	n/a	30.77	30770	n/a	30.83	30830	n/a	30.62	30620	n/a							
Chemical Critical Point temperature (ambient pressure)	K	525.6552198	5.2300E+02	n/a	2 values the same from a consistent range.	Average	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a										
						523	523.00	n/a	523	523.00	n/a	no data	#VALUE!	n/a	523.4	523.40	n/a	523.4	523.40	n/a	523.4	523.40	n/a	523.4	523.40	n/a	523.4	523.40	n/a	523.4	523.40	n/a	523.4	523.40	n/a							
Critical Pressure	atm	49.28559298	50.03	not given	2 values across consistent range. Value from most recent source chosen.	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a										
						50.7	50.03700962	n/a	50.7	50.03700962	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a	50.61	49.9481865	n/a							

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	1.29E-01	10	Estimated from parameters above using Clayton relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	1.545E+04	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	8.73E-06	10	Estimated from parameters above using Wilke-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	6.74E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	1.55	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

1,1-Dichloroethene	CAS Number: 75-35-4	Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF
		Date: 08/04/2009	Date: 29/04/2009	Date: 25/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Insufficient data to assess non-threshold effects, HCV based on threshold effects.
Apply IDoral to exposure routes?	No	No	No		
Apply TDinh to exposure routes?	No	No	Yes		Insufficient data to assess non-threshold effects, HCV based on threshold effects.
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	46	ug.kg-1.d-1	46 (or round to 50) as consensus value from the majority of sources (WHO, US EPA IRIS, CICADs). RIVM value discounted as it is provisional and based on route to route extrapolation; ATSDR value discounted as based on 1992 IRIS recommendation which has subsequently been revised.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Agency for Research on Cancer (IARC)	<a href="http://incem.org/pages/iarc.html">http://incem.org/pages/iarc.html</a>	13/04/1999	16/03/2009										
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://incem.org/pages/cicads.html">http://incem.org/pages/cicads.html</a>	2003	20/03/2009	TDI	0.05 (rounded up from 0.046)	mg.kg-1.d-1	50	Uncertainty that the lab animal data have demonstrated the correct target tissue for humans	BMD10	4.6	mg.kg-1.d-1	100	10 interspecies and 10 intraspecies
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://incem.org/pages/ehc.html">http://incem.org/pages/ehc.html</a>	1990	20/03/2009	Not given	Not given								
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/en">http://www.who.int/water_sanitation_health/dwa/guidelines/en</a>	2006	16/03/2009	TDI	0.046	mg.kg-1.d-1	46	Not given	BMD	Not given		Not given	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	1998	20/03/2009	Oral Max. Permissible Risk MPR TDI	3	ug.kg-1bw-1.d-1	3	Provisional value (tentative value based on route to route extrapolation)	Not given				None
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	2005	20/03/2009							5	mg.kg-1.d-1	Not given	LOAEL
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	May-94	16/03/2009	RfD	0.009	mg.kg-1.d-1	9	Not given; based on now superseded IRIS recommendation	LOAEL	9	mg.kg-1.d-1	1000	10 interspecies, 10 intraspecies, 10 LOAEL to NOAEL
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	13/08/2002	16/03/2009	RfD	5.0 x10-2	mg.kg-1.d-1	50	Medium	BMDL10	4.6	mg.kg-1.d-1	100	10 interspecies, 10 intraspecies

## 1,1-Dichloroethene

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
International Agency for Research on Cancer (IARC)		Not classifiable as to its carcinogenicity to humans (Group 3)			<a href="http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html">http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html</a>
IPCS concise International Chemical Assessment Documents (CICADs)	Oral exposure	Female rat study	Minimal hepatocellular midzonal fatty change	Quast, JF; Humiston, CG; Wade, CE; et al. (1983) A chronic toxicity and oncogenicity study in rats and subchronic toxicity study in dogs on ingested vinylidene chloride. Fundam Appl Toxicol 3:55-62.	<a href="http://inchem.org/documents/cicads/cicads/cicad51.htm#11.1">http://inchem.org/documents/cicads/cicads/cicad51.htm#11.1</a>
IPCS Environmental Health Criteria (EHC) Monographs		Oral dosing of rats for one year with up to 30 mg/kg daily	Minimal hepatic changes	Not given	<a href="http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4">http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4</a>
WHO Guidelines for drinking water Quality		Female rat study	hepatocellular midzonal fatty change	Not indicated, presumably this is Quast et al. 1983	<a href="http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels					<a href="http://www.rivm.nl/bibliotheek/rapporten/711701005.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701005.pdf</a>
Health Canada Toxicological Values	Chronic duration oral exposure	Two year gavage study in male and female rats	Chronic renal inflammation	NTP (National Toxicology Program). 1982. Carcinogenesis bioassay of vinylidene chloride (CAS No. 75-35-4) in F344 rats and B6C3F1 mice (gavage study). National Toxicology Program, Research Triangle Park, North Carolina (Technical Report Series No. 228; PB	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Chronic duration oral exposure	Rats were exposed to 50 ppm 1,1-dichloroethene (converted by the investigators to a dose of 9 mg/kg/day based on body weight and water consumption data) in utero, during lactation, and through weaning into adulthood over a period of over 365 days.	Hepatocellular changes (liver effects)	Quast, JF; Humiston, CG; Wade, CE; et al. (1983) A chronic toxicity and oncogenicity study in rats and subchronic toxicity study in dogs on ingested vinylidene chloride. Fundam Appl Toxicol 3:55-62.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp39.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp39.pdf</a>
USEPA Integrated Risk Information System (IRIS)	2 year chronic toxicity and carcinogenicity study	1,1-DCE was incorporated into the drinking water of male and female rats at concentrations of 0,50,100 or 200 ppm.	hepatocellular midzonal fatty change	Quast, JF; Humiston, CG; Wade, CE; et al. (1983) A chronic toxicity and oncogenicity study in rats and subchronic toxicity study in dogs on ingested vinylidene chloride. Fundam Appl Toxicol 3:55-62.	<a href="http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf">http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf</a>

1,1-Dichloroethene		CAS Number: 75-35-4		Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF							
				Date: 08/04/2009	Date: 29/04/2009	Date: 25/08/2009							
TDI inhal				Recommended TDIinhal	Units	Justification							
				57	ug.kg-1.d-1	Majority consensus (CICADs, RIVM, US EPA IRIS). ATSDR recommended a lower value in an older study which has not been recommended due majority consensus from most recent sources.							
Organisation		Last Updated		Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	13/04/1999	19/03/2009										
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	2003	20/03/2009	Tolerable Concentration in Air TCA	0.2	mg.m3	57	Not given	BMCL HEC (Human Equivalent Concn)	6.9	mg.m3		30 3 for interspecies because a dosimetric adjustment was used 10 intraspecies
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1990	20/03/2009	Not given	Not given								
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Oct-93	20/03/2009	Maximum Permissible Concentration in air, MPC	200	ug.m3	57	Not given	NOAEL	20	mg.m3		100 10 interspecies, 10 intraspecies
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	Nov-05	20/03/2009						LOAEC (concn)	40	mg.m3	Not given	Not given
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	May-94	16/03/2009	Inhalation MRL (conversion: 1ppm = 4.0mg/m <sup>3</sup> )	0.02 ppm [conv = 0.08 mg/m <sup>3</sup> ]	ppm	22.8	Not given	NOAEL	5	ppm	Not given	Not given
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	13/08/2002	16/03/2009	RfC	0.2	mg/m3	57	Medium	BMCL 10HEC	6.9	mg/m3		30 3 for interspecies extrapolation 10 for intraspecies variability

## 1,1-Dichloroethene

TDI inhal					
Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)		Vinylidene chloride is not classifiable as to its carcinogenicity to humans (Group 3).			<a href="http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html">http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html</a>
IPCS concise International Chemical Assessment Documents (CICADs)	Chronic inhalation study	Female rat study	Minimal hepatocellular midzonal fatty change	Quast, JF; Mckenna, MJ; Rampy, LW; et al. (1986) Chronic toxicity and oncogenicity study on inhaled vinylidene chloride in rats. Fundam Appl Toxicol 6:105-144.	<a href="http://inchem.org/documents/cicads/cicads/cicad51.htm#11.1">http://inchem.org/documents/cicads/cicads/cicad51.htm#11.1</a>
IPCS Environmental Health Criteria (EHC) Monographs	Long term inhalation study	Rats subject to intermittent exposure	Mild reversible hepatic changes at an exposure level of 300 mg/m3 in rats	Not given	<a href="http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4">http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Intermediate duration inhalation exposure	Groups of rats, guinea pigs, rabbits, dogs and monkeys were continually exposed to 0, 20, 61, 101 or 189 mg.m3 for 90 days	Mortality rates increased, body weights decreased and there were histopathological changes at doses of 62 mg.m3 and above	Prendergast JA, Jones RA, Jenkins LJ, et al. 1967. Effects on experimental animals of long-term inhalation of trichloroethylene, carbon tetrachloride, 1,1,1-trichloroethane, dichlorodifluoromethane, and 1,1-dichloroethylene. Toxicol Appl Pharmacol 10:270-	<a href="http://www.rivm.nl/bibliotheek/rapporten/679101010.pdf">http://www.rivm.nl/bibliotheek/rapporten/679101010.pdf</a>
Health Canada Toxicological Values	long duration inhalation exposure	52 week study of male swiss mice	significant increases in kidney damage	Maltoni, C., Cotti, G. and Chieco, P. 1984. Chronic toxicity and carcinogenicity bioassays of vinylidene chloride. Acta Oncol. 5: 91-146 [cited in IPCS, 1990].	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Intermediate duration Inhalation exposure	Guinea pigs were exposed to 5, 15, 25, or 48 ppm of 1,1-dichloroethene for 24 hours per day for 90 days	Liver effects. Mottled livers within the 15 ppm group	Prendergast JA, Jones RA, Jenkins LJ, et al. 1967. Effects on experimental animals of long-term inhalation of trichloroethylene, carbon tetrachloride, 1,1,1-trichloroethane, dichlorodifluoromethane, and 1,1-dichloroethylene. Toxicol Appl Pharmacol 10:270-	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp39.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp39.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Chronic Inhalation study	Male and female rats were exposed to 1,1-DCE by inhalation 6 hrs/day, 5 days/week for up to 18 months. Rats were exposed to concentrations of 10 ppm and 40 ppm for the first five weeks and then 25 ppm and 75 ppm for the rest of the time	Minimal hepatocellular midzonal fatty change	Quast, JF; Mckenna, MJ; Rampy, LW; et al. (1986) Chronic toxicity and oncogenicity study on inhaled vinylidene chloride in rats. Fundam Appl Toxicol 6:105-144.	<a href="http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf">http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf</a>

1,1-Dichloroethene	CAS Number: 75-35-4	Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF
		Date: 08/04/2009	Date: 29/04/2009	Date: 25/08/2009

ID oral	Recommended IDoral	Units	Justification
	none		Insufficient data

Organisation		Last Updated		Non threshold effects?	Basis	Health criteria type	Value	Units		Confidence rating			Basis
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	13/04/1999	29/04/2009	Vinylidene chloride is not classifiable as to its carcinogenicity to humans (Group 3).									
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	2003	29/04/2009	Fairly extensive database on the genotoxicity									
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1990	29/04/2009	Genotoxicity has been observed in prokaryotic and eukaryotic cells in vitro. However, genotoxicity was not observed in the majority of tests carried out on mammals in vivo.	Not given								
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	2005	29/04/2009	the weight of evidence for carcinogenicity and genotoxicity is limited, a mode of action for induction of effects involving direct interaction with genetic material cannot be precluded.									
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	May-94	29/04/2009	No studies were located regarding genotoxic effects in humans or animals after oral exposure									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/06/2002	29/04/2009	None of the bioassays by the oral route of exposure provide sufficient evidence that 1,1-DCE is a carcinogen									

## 1,1-Dichloroethene

ID oral					
Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)		Vinylidene chloride is not classifiable as to its carcinogenicity to humans (Group 3).			<a href="http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html">http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html</a>
IPCS concise International Chemical Assessment Documents (CICADs)					<a href="http://www.inchem.org/documents/cicads/cicads/cicad51.htm">http://www.inchem.org/documents/cicads/cicads/cicad51.htm</a>
IPCS Environmental Health Criteria (EHC) Monographs					<a href="http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4">http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4</a>
Health Canada Toxicological Values					
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels					
USEPA Integrated Risk Information System (IRIS)					<a href="http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf">http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf</a>

1,1-Dichloroethene	CAS Number: 75-35-4	Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF
		Date: 08/04/2009	Date: 29/04/2009	Date: 25/08/2009

ID inhal	Recommended IDinhal	Units	Justification
	none		Insufficient data

Organisation		Last Updated		Non threshold effects?	Basis	Health criteria type	Value	Units		Confidence rating			Basis
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	13/04/1999	29/04/2009	Vinylidene chloride is not classifiable as to its carcinogenicity to humans (Group 3).									
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	2003	29/04/2009	Fairly extensive database on the genotoxicity									
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1990	29/04/2009	Genotoxicity has been observed in prokaryotic and eukaryotic cells in vitro. However, genotoxicity was not observed in the majority of tests carried out on mammals in vivo.	Not given								
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Oct-93	29/04/2009	Mutagenic to bacteria; no chromosomal aberration in mammalian cells; DNA damage observed in mammalian cells; limited evidence for carcinogenicity in animals, inadequate evidence to humans.									
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	May-94	29/04/2009	Several in vitro studies suggest that 1,1-dichloroethene, only in the presence of activating systems, is mutagenic in both prokarydc and eukatydc organisms. These results are consistent with the idea that a reactive metabolic intermediate(s), and not the									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/06/2002	29/04/2009	One bioassay by the inhalation route of exposure showed suggestive evidence of carcinogenicity for humans. EPA does not currently believe that the suggestive evidence of a tumor response provides sufficient weight of evidence to justify deriving an inhalation									

## 1,1-Dichloroethene

ID inhal					
Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)		Vinylidene chloride is not classifiable as to its carcinogenicity to humans (Group 3).			<a href="http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html">http://www.inchem.org/documents/iarc/vol71/050-vinylchl.html</a>
IPCS concise International Chemical Assessment Documents (CICADs)					<a href="http://www.inchem.org/documents/cicads/cicads/cicad51.htm">http://www.inchem.org/documents/cicads/cicads/cicad51.htm</a>
IPCS Environmental Health Criteria (EHC) Monographs					<a href="http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4">http://inchem.org/documents/ehc/ehc/ehc100.htm#SubSectionNumber:1.4.4</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels					<a href="http://www.rivm.nl/bibliotheek/rapporten/679101010.pdf">http://www.rivm.nl/bibliotheek/rapporten/679101010.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels					
USEPA Integrated Risk Information System (IRIS)					<a href="http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf">http://www.epa.gov/ncea/iris/toxreviews/0039-tr.pdf</a>

1,1-Dichloroethene	CAS 75-35-4	Assessor A: Cheryl Davies, De	Assessor B: Siân Jones, Entec	Final Review:	Panel/SF
		Date: Mar-09	Date: 29-Apr-09	Date:	25/08/2009

MDI	Recommended MDIoral	Units	Justification: Calculated for a 70 kg adult drinking 2 litres of water per day, from mean concentration within drinking water of 0.003 mg.L-1 (IPCS CICADS)
	6	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
International Agency for Research on Cancer (IARC)	1990	Drinking water	20	ug litre-1	Maximum level reported in drinking water (US)	Not given but is within <a href="http://www.inchem.org/documents/ehc/ehc/ehc100.htm">http://www.inchem.org/documents/ehc/ehc/ehc100.htm</a>	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	2003	Drinking water	6 to 9x10 <sup>-5</sup>	mg.kg bw-1.d-1	Calculated for a 70 kg adult drinking 2 litres of water per day, from mean concentration within drinking water of 0.002 to 0.003 mg.litre-1. The oral exposure from food and soil is most likely negligible	<a href="http://inchem.org/documents/cicads/cicads/cicad51.htm#11.1">http://inchem.org/documents/cicads/cicads/cicad51.htm#11.1</a>	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
IPCS Environmental Health Criteria (EHC) Monographs	1990	Drinking water	<0.01	ug day-1	Estimate of Average daily exposure of USA citizens Maximum level reported in drinking water 20 ug.litre-1	<a href="http://www.inchem.org/documents/ehc/ehc/ehc100.htm#SectionNumber:10.2">http://www.inchem.org/documents/ehc/ehc/ehc100.htm#SectionNumber:10.2</a>	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>
WHO Guidelines for Drinking Water Quality	2006	Drinking water No data on levels within food	0.5	ug litre -1	Concentrations within public drinking water supplies <0.2 to 0.5 ug litre-1	WHO. 2006. Guidelines for drinking-water quality. First Addendum to Third Edition. Recommendations. Geneva, Switzerland: World Health Organization.	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">www.who.int/water_sanitation_health/dwg/guidelines/en</a>
WHO Air Quality Guidelines for Europe	2005	No information here on 1,1-DCE					<a href="http://www.euro.who.int/air/activities/20050222_2">www.euro.who.int/air/activities/20050222_2</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	1998	Estimated background exposure	0.014	ug.kg bw-1.d-1	No further detail	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701005.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701005.pdf</a>	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
Health Canada Toxicological Reference Values	2005	Food and beverages and drinking water	0.0191	ug.kg bw-1.d-1	Assumes 0.017 ug.kg bw-1.d-1 from food and beverages and 0.0021 ug.kg bw-1.d-1 drinking water for adult aged 20-59 years, 70 kg, based on UK food intake concentrations (MAFF, 1980)	<a href="http://www.hc-sc.gc.ca/ewh-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf">http://www.hc-sc.gc.ca/ewh-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf</a>	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	May-94	Drinking water	0.3	ug litre-1	Guideline for drinking water quality (This has now been superseded in 3rd edition. Now	WHO. 1984. Guidelines for drinking-water quality. Recommendations. Geneva, Switzerland:	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
USEPA Health Advisories	Page Last updated 18/03/2009	Drinking water	0.007	mg.litre-1	Maximum contaminant Level MCL allowed in Drinking water in the US, due to liver problems	<a href="http://www.epa.gov/safewater/contaminants/index.html">http://www.epa.gov/safewater/contaminants/index.html</a>	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
Toxicological Data Network (TOXNET)	HSDB Last reviewed 15/09/2001	Drinking water	78	ug litre-1	Maximum concentration identified within California public drinking water wells sampled during 1984 and 1990. Was present within 72 wells out of 7712	Lam RHF et al, pp. 15-44 in Water Contamination and Health. Wang RGM, ed. NY, NY: Marcel Dekker (1994)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

1,1-Dichloroethene	CAS 75-35-4	Assessor A: Cheryl Davies, De	Assessor B: Siân Jones, Entec	Final Review: Panel/SF
		Date: Mar-09	Date: 29-Apr-09	Date: 25/08/2009
<b>MDI</b>		<b>Recommended MDI<sub>inh</sub></b> 0.4	<b>Units</b> ug day <sup>-1</sup>	Justification: Based on median urban air concentrations in the USA for non-industrial source area of 20 ng/m <sup>3</sup> (EHC Monographs). Converted to MDI of 0.4 ug/d (20 ng/m <sup>3</sup> x 20 m <sup>3</sup> /d / 1000 ng/ug).

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Health and Safety Executive	2005	Air	40	mg.m-3 over 8 hr TWA	Vinylidene Chloride Long term Occupational Exposure Limit 10 ppm or 40 mg.m-3 over 8 hr TWA (workplace exposure, not typical background)	EH40/2005 <a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>	<a href="http://www.hse.gov.uk">www.hse.gov.uk</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	2003	Air	4	µg.m-3	Upper end of the range for the mean concentration of 1,1-DCE in air will not exceed 0.004 mg/m <sup>3</sup> (equivalent to MDI <sub>inh</sub> of 80µg/day)	US EPA (2002a) AirData. Washington, DC, US Environmental Protection Agency, at website <a href="http://www.epa.gov/aqspubl1/annual_summary.html">http://www.epa.gov/aqspubl1/annual_summary.html</a> .	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
IPCS Environmental Health Criteria (EHC) Monographs	1990	Air	8.7	µg.m-3	Median urban air concentrations in the USA for non-industrial source area is 20 ng/m <sup>3</sup> . Median for industrial is 8.7 ug.m <sup>3</sup> (equivalent to MDI <sub>inh</sub> of 174µg/day)	US EPA (1985) Health assessment document for vinylidene chloride, Washington, DC, US Environmental Protection Agency, Office of Health and Environmental Assessment (EPA 600/8-83-031F).	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>
Health Canada Toxicological Reference Values	2005	Indoor Air	0.81	ug.kg bw <sup>-1</sup> .d <sup>-1</sup>	Estimated adult indoor air inhalation intake, assuming age 20-59, weight 70 kg and breathes 16.2 m <sup>3</sup> air.day <sup>-1</sup> and spends 21 hours per day indoors. Based on Canadian study of indoor air within 75 houses in Ottawa by Health Canada, 2003. (equivalent to MD	<a href="http://www.hc-sc.gc.ca/ewh-scem/alt_formats/hecs-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf">http://www.hc-sc.gc.ca/ewh-scem/alt_formats/hecs-sesc/pdf/pubs/contaminants/dichloroethene/dichloroethene-eng.pdf</a>	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	May-94	Ambient Air	6.5	ug m-3	Average background exposure to the general population (U.S) based on air samples from 350 homes in New Jersey (equivalent to MDI <sub>inh</sub> of 130µg/day)	Wallace LA. 1991. Comparison of risks from outdoor and indoor exposure to toxic chemicals. Environ Health Perspect 95:7-1X	<a href="http://atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
Toxicological Data Network (TOXNET)	HSDB Last reviewed 15/09/2001	Ambient Air	3800	parts per trillion	Mean concentration of 14 samples from the USA, location unspecified (equivalent to a concentration of 15.2µg/m <sup>3</sup> , or an MDI of 304µg/day)	Brodzinsky R, Singh HB; Volatile Organic Chemicals in the Atmosphere: An Assessment of Available Data. SRI Inter Contract 68-02-3452. pp. 198 (1982)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

Substance:		1,1-Dichloroethene		CAS Number:		75-35-4		Assessor A:		Jennifer Stothert, Entec		Assessor B:		Cheryl Davies, Delta-Simons		Final Review:		Panel/SF																	
Chemical Formula:		C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> (CH <sub>2</sub> =CCl <sub>2</sub> )		Phase at Ambient Temperature		Liquid		Date:		11-Mar-09		Date:		16-Apr-09		Date:		25-Aug-09																	
																		<a href="http://srdata.nist.gov/solubility/">http://srdata.nist.gov/solubility/</a> <a href="http://webbook.nist.gov/chemistry/">http://webbook.nist.gov/chemistry/</a> <a href="http://cs3-hq.oecd.org/scripts/hpw/">http://cs3-hq.oecd.org/scripts/hpw/</a>																	
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H							
							HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCX, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000							
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)					
<b>Required Parameters</b>																																			
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	96.9427	n/a	Median value chosen as central value of consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)					
Average							96.950	96.950	n/a	96.943	96.943	n/a	96.943	96.943	n/a	96.940	96.940	n/a	96.940	96.940	n/a	96.940	96.940	n/a	96.9427	96.9427	n/a	96.940	96.940	n/a					
Geomean							3.01E-02	3.05E+03	25	2.62E+00	2.62E+03	25	3.73E+03	3.729	25	2.82E+03	25	n/a	n/a	n/a	1.50E-02	1519.875	25	3.40E-02	2.95E+03	25	3.40E-02	2.95E+03	25	2.29E-01	23200	20			
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	2.62E+03	25	No consistent range - median value from most recent review chosen (Lide 2008)		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)					
Geomean							3.01E-02	3.05E+03	25	2.62E+00	2.62E+03	25	3.73E+03	3.729	25	2.82E+03	25	n/a	n/a	n/a	1.50E-02	1519.875	25	3.40E-02	2.95E+03	25	3.40E-02	2.95E+03	25	2.29E-01	23200	20			
Average							3.01E-02	3.05E+03	25	2.62E+00	2.62E+03	25	3.73E+03	3.729	25	2.82E+03	25	n/a	n/a	n/a	1.50E-02	1519.875	25	3.40E-02	2.95E+03	25	3.40E-02	2.95E+03	25	2.29E-01	23200	20			
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Contaminant Name: 1,2,4-Trimethylbenzene	CAS Number: 95-63-6	Assessor A: Mathew Rouge	Assessor B: Gareth Wills	Final Review: Panel/SF
Date: Mar-09		Date: Apr-09	Date: 28/08/2009	

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	Yes	Route-to-route extrapolation from inhalation to oral and dermal routes. No information available regarding carcinogenicity
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	Yes	Yes	Yes		TDlinh applied to inhalation route. No information available regarding carcinogenicity
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	none	ug.kg-1.d-1	No recommended TDloral, insufficient data with sufficient detail on derivation to derive. Use route-to-route extrapolation from inhalation.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2009	Jul-09	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Office of Environmental Health Hazard Assessment	<a href="http://oehha.ca.gov/water/pals/124135tmb.html">http://oehha.ca.gov/water/pals/124135tmb.html</a>	2001	Jul-09	Sub chronic RfD	47.66	ug/kg bw/day	47.66	Not provided	NOAEL	143	mg/kg-day	3000	10 for interspecies extrapolation, 10 for extrapolation from subchronic to chronic study, 10 for human variability, 3 for database deficiencies.	Subchronic rat study
Risk Assessment Information System	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>	2008	Mar-09	RfD	50	ug/kg bw/day	50	Low	NOAEL	Not provided	Not provided	3000	Not provided	rat
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>	2008	Mar-09	RfD	50	ug/kg bw/day	50	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	No info.

TDI inhal	Recommended TDlinhal	Units	Justification
	2	ug.kg-1.d-1	TDIinhalation based upon provisional RfC. Korsak (2000) study is the primary source, with supporting information from Korsak et al (1997) and Battig et al (1958).

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	2007	Mar-09	Workplace Exposure Limit	125 (All trimethylbenzene isomers)	mg/m3	35714.29 ug/kg bw/day	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2007	Jul-09	p-RfC	7.00E-03	mg/m3	2 ug/kg bw/d	low	NOAEL	21.8	mg/m3	3000	10 for subchronic to chronic extrapolation, 3 for animal to human extrapolation, 10 for interindividual variability and 10 for database deficiencies	subchronic rat study
Risk Assessment Information System	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>	2008	Mar-09	RfC	7.00E-03	mg/m3	2 ug/kg bw/d	low	NOAEL	21.8	mg/m3	3000	No details provided	Human study
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>	2008	Mar-09	RS-ESL	6.00E-03	mg/m3	1.71 ug/kg bw/d	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided

ID oral	Recommended IDoral	Units	Justification
	N/A		No information available regarding carcinogenicity

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2007	Jul-09	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

ID inhal	Recommended IDinhal	Units	Justification
	N/A		No information available regarding carcinogenicity

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
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**Contaminant Name:1,2,4-Trimethylbenzene**

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	The database for 1,2,4-trimethylbenzene is inadequate to derive a provisional RfD	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>
Office of Environmental Health Hazard Assessment	Groups of 10 male and 10 female Sprague-Dawley rats were administered 1,3,5-TMB by gavage in corn oil.	Abnormal clinical observations consisted of discoloured and/or wet inguinal fur and salivation in the highest dose group of both sexes. Critical effects included increases in mean absolute liver weight and mean relative kidney weight.	IITRI (1995). 90-Day oral gavage toxicity study of 1,3,5-trimethylbenzene in rats with a recovery group. Industry Institute of Toxicology Research Institute. Study conducted for Koch Industries Inc., Wichita, KS.	<a href="http://oehha.ca.gov/water/pals/124135tmb.html">http://oehha.ca.gov/water/pals/124135tmb.html</a>
Risk Assessment Information System	Not provided	dec in body wt gain; clinical observations; inc liver/kidney wt in rats	IITRI (1995). 90-Day oral gavage toxicity study of 1,3,5-trimethylbenzene in rats with a recovery group. Industry Institute of Toxicology Research Institute. Study conducted for Koch Industries Inc., Wichita, KS.	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>
Texas Commission on Environmental Quality	The value is provided by the US EPA National Centre for Environmental Assessment (NCEA)	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>
TDI inhal				
Organisation	Description	Response	Reference	Web link
Health and Safety Executive (HSE)	8 hour long term workplace exposure limit	Not provided	Not provided	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	male and female rats exposed to 97% pure 1,2,4-tmb. Battig et al (1958) and Korsak et al (1997) provide supporting evidence.	decreased clotting time in female rats	Korsak et al, 2000. sub-chronic inhalation toxicity of 1,2,4-trimethylbenzene (speudocumene) in rats. Int. J. Occup. Med. Environ. Health. 13(2):155-164	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>
Risk Assessment Information System	Not provided	CNS effects, asthma-like bromchitis, aneima, blood clot effects	Battig et al 1958	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>
Texas Commission on Environmental Quality	The value is provided by the US EPA National Centre for Environmental Assessment (NCEA)	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>
ID oral				
Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	There are no appropriate human or animal data from which to derive an oral slope factor	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>
ID inhal				
Organisation	Description	Response	Reference	Web link

<b>1,2,4-Trimethylbenzene</b>	95-63-6	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
		Date	08/04/2009	Date	15/04/2009	Date	28/08/2009

MDI	<b>Recommended MDIoral</b>	<b>Units</b>	Justification: Only literature value obtained. Conservative, based upon maximum recorded concentration in tap water (US National Tap Water Quality Database). Converted assuming 2L/d consumed.
	24	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Other - National Tap Water Quality Database		tap water	Max concentration in tap water 12ppb	24 ug/d (assuming 2litres of water/d)	value taken from highest recorded concentration in tap water, US. Converted to daily intake assuming 2 litres of water consumed per day.	National Tap Water Quality Database	<a href="http://www.ewg.org/tapwater/contaminants/contaminant.php?contamcode=2418">http://www.ewg.org/tapwater/contaminants/contaminant.php?contamcode=2418</a>

MDI	<b>Recommended MDIinh</b>	<b>Units</b>	Justification: only literature value obtained (TOXNET)
	86	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Toxicological Data Network (TOXNET)	1985	Ambient Air	86	ug day-1	The average daily dose of 1,2,4-trimethylbenzene from breathing air in The Netherlands was estimated as 86 ug/day based on average ambient air concentrations of 0.50-1.15 ppb (conversion not detailed within Toxnet - but is assumed to be approximately $1.15e-9 \times 1 \text{ atm} \times 120.19 \text{ g.mol}^{-1} \times 15 \text{ m}^3.\text{d}^{-1} \times 1e6 \text{ ug.g}^{-1} / (8.206e-5 \text{ atm.m}^3.\text{mol}^{-1}.\text{K}^{-1} \times 288 \text{ K})$ )	Guicherit R, Schulting FL; Sci Total Environ 43: 193-219 (1985)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

Substance:	<b>1,2,4-Trimethylbenzene (Pse)</b>	CAS Number:	95-63-6	Assessor A:	Mathew Rouge	Assessor B:	Gareth Wills	Final Review:	Panel/SF
Chemical Formula:	C9H12	Phase at Ambient Temperature:	Liquid	Date:	25/03/2009	Date:	30/04/2009	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oecd.org/scripts/hpv/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A		B		C		D		E		F		G		H									
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)			
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	120.191	n/a	All values the same	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
							No info.	#VALUE!	n/a	120.191	120.191	n/a	120.191	120.191	n/a	120.191	120.191	n/a	120.191	120.191	n/a	120.191	120.191	n/a	120.191	120.191	n/a	120.191	120.191	n/a
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	5.69E+02	25	Values not in consistent range, therefore value taken from most recent reference	Geomean	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
							No info.	#VALUE!	25	5.69E+02	5.69E+02	25	7.04E+02	7.04E+02	27	n/a	n/a	n/a	6.95E-03	704.20875	27	No info.	#VALUE!	25	1.50E-01	6.69E+02	25	No info.	#VALUE!	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	5.59E+02	25	Central value from consistent range selected	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
							No info.	#VALUE!	n/a	5.70E-02	57	n/a	5.70E+01	5.70E+01	n/a	No info.	#VALUE!	n/a	5.19E+01	5.19E+01	25	No info.	#VALUE!	n/a	5.70E+01	5.70E+01	25	No info.	#VALUE!	n/a
Chemical Boiling Point (ambient pressure)	K	n/a	4.43E+02	n/a	Central value from consistent range selected	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	K	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							No info.	#VALUE!	n/a	169.38	442.53	n/a	169.38	442.53	n/a	170	443.15	n/a	169.3	442.45	n/a	No info.	#VALUE!	n/a	442.4	442.40	n/a	169	442.15	n/a
Chemical Melting Point (ambient pressure)	K	n/a	2.29E+02	n/a	Central value from consistent range selected	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	K	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							No info.	#VALUE!	n/a	-43.77	229.38	n/a	-43.77	229.38	n/a	-43.78	229.37	n/a	-43.8	229.35	n/a	No info.	#VALUE!	n/a	229.33	229.33	n/a	-44	229.15	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	3.76	n/a	Central value from consistent range selected.	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
							No info.	No info.	n/a	3.63	3.63	n/a	3.65	3.65	n/a	No info.	No info.	n/a	3.55	3.55	n/a	No info.	No info.	n/a	No info.	No info.	n/a	3.8	3.80	n/a
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	1.63E+02	n/a	Single value selected	Average	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	39089.08948	3.91E+04	Normal Boiling Point	Calculated value chosen	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Chemical Critical Point temperature (ambient pressure)	K	654.2376286	6.54E+02	n/a	Calculated value chosen - this is similar to range of reported values	Average	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Critical Pressure	atm	31.77087119	3.18E+01	n/a	Calculated value chosen - this is similar to range of reported values	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale	Property	Units	Calculated Value	Ref. Temp (C)	Rationale	Property	Units	Calculated Value	Ref. Temp (C)	Rationale	Property	Units	Calculated Value	Ref. Temp (C)	Rationale					
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	8.562E-02	10	Estimated from parameters above using Clapryon relationship or direct calculation	Vapour pressure at ambient soil temperature	Pa	110.348996	10	Estimated from parameters above using Grain-Watson method	Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	6.44E-06	10	Estimated from parameters above using Wilkie-Lee method	Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	4.87E-10	10	Estimated from parameters above using Hayduk and Laudie method	Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	3.15	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

<b>1,2-Dichloropropane</b>	<b>CAS Number:</b> 78-87-5	<b>Assessor A:</b> J Lymer, Wardell Armstrong	<b>Assessor B:</b> D Brooks, Sirius	<b>Final Review:</b> Panel/SF
		Date: 13/03/2009	Date: 14/04/2009	Date: 28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Group 3 carcinogen (IARC), not classifiable as to its carcinogenicity to humans - TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		Group 3 carcinogen (IARC), not classifiable as to its carcinogenicity to humans - TDlinh applied to inhalation routes
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	14	ug.kg-1.d-1	WHO most appropriate value as this is the only fully referenced value

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	Sep-02	13/03/2009	No health criteria value data										Genotoxicity in rodents	1,2-Dichloropropane was a likely candidate in producing potential genotoxicity as a component of a pesticide
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	1999	13/03/2009	No health criteria value data											There is limited evidence in experimental animals for the carcinogenicity of 1,2-dichloropropane. No evaluation of the carcinogenicity of 1,2-dichloropropane to humans could be made.
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1993	13/03/2009	No chronic health criteria value											
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2003	13/03/2009	Oral TDI	14	ug/kg/day	14	N/A	LOAEL	71.4	mg/kg/day	5000	100 for inter- and intraspecies variation, 10 for the use of a LOAEL instead of a NOAEL, and 5 for limitations of the database, including the limited data on in vivo genotoxicity and use of a subchronic study	Reproductive and development (testicular) toxicity	13 week toxicity study in which male rats were administered with 1,2-DCP by gavage in corn oil for 5days/week
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Original December 1989 and published as MRL December 2008	13/03/2009	Oral chronic MRL	0.09	mg/kg/day	90	N/A				1000			
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/12/1991	13/03/2009	No health criteria value data											

TDI inhal	Recommended TDlinhal	Units	Justification
	1.14	ug.kg-1.d-1	Only available value from reliable source (IRIS) chosen

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	30/11/2003	15/07/2009	No health criteria value data										Mice study	80 C3H mice exposed 37 times to 400ppm for 4-7 hrs over 7 months.
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/12/1991	13/03/2009	Inhalation RFC	4.00E-03	mg/m3	1.14E+00	Medium	LOAEL	1.3	mg/m3	300	The uncertainty factor of 300 reflects a factor of 10 to protect sensitive individuals. A factor of 3 is used for extrapolation from a subchronic study, since study of the critical effect shows little progression with exposure time. A factor of 3 is used for the use of a minimal LOAEL due to the minimal nature of the effect. A factor of 3 is used for interspecies extrapolation due to the use of dosimetric adjustments.	Mice study	Male and female mice were exposed to 1,2-DCP for 6 hours per day, 5 days/week for 13 weeks.

Recommended IDoral															
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type	Description			
Recommended IDinhal															
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type	Description			

**1,2-Dichloropropane****TDI oral**

Organisation	Target organ/Critical Effect	Reference	Web link
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	Cytogenetic abortions	Risk Assessment of Mixtures of Pesticides and Similar Substances	<a href="http://cot.food.gov.uk/pdfs/reportindexed.pdf">cot.food.gov.uk/pdfs/reportindexed.pdf</a>
International Agency for Research on Cancer (IARC)			<a href="http://incem.org/documents/iarc/vol71/084-12dichprop.html">http://incem.org/documents/iarc/vol71/084-12dichprop.html</a>
IPCS Environmental Health Criteria (EHC) Monographs		Environmental Health Criteria 146	<a href="http://incem.org/documents/ehc/ehc/ehc146.htm">http://incem.org/documents/ehc/ehc/ehc146.htm</a>
WHO Guidelines for drinking water Quality	Testicular degeneration and in increased number of degenerate spermatogonia in the epididymis	1,2-Dichloropropane (1,2-DCP) in Drinking-water Background document for development of WHO Guidelines for Drinking-water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/1,2-Dichloropropane.pdf">http://www.who.int/water_sanitation_health/dwg/1,2-Dichloropropane.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Hepatic	Agency for Toxic Substances and Disease Registry (ATSDR) U.S. Public Health Service, In collaboration with U.S. Environmental Protection Agency (EPA) December 1989. TOXICOLOGICAL PROFILE FOR 1,2-DICHLOROPROPANE	<a href="http://www.atsdr.cdc.gov/substances/toxsubstance.asp?toxid=162">http://www.atsdr.cdc.gov/substances/toxsubstance.asp?toxid=162</a>
USEPA Integrated Risk Information System (IRIS)			<a href="http://www.epa.gov/ncea/iris/subst/0601.htm">http://www.epa.gov/ncea/iris/subst/0601.htm</a>

**TDI inhal**

Organisation	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Necrotic liver lesions. Study inadequate - not feasible to derive PPRTV	Heppel, L.A., B. Highman and E.G. Peake. 1948. Toxicology of 1,2-dichloropropane (propylene bichloride) IV. Effects of repeated exposures to a low concentration of the vapour. J. Ind Hyg. Toxicol. 30: 189-191	
USEPA Integrated Risk Information System (IRIS)	LOAEL is based on nasal epithelial hyperplasia in female rats	Nitschke K.D., K.A. Johnson, D.L. Wackerle, J.E. Phillips and D.A. Dittenber. 1988. Propylene dichloride: A 13-week inhalation toxicity study with rats, mice, and rabbits. Dow Chemical Company, Mammalian and Environmental Toxicology Research Laboratory, Midland, MI. OTS Doc. #86-870001397	<a href="http://www.epa.gov/ncea/iris/subst/0601.htm#refinhal">http://www.epa.gov/ncea/iris/subst/0601.htm#refinhal</a>

**ID oral**

Organisation	Response	Reference	Web link

**ID inhal**

Organisation	Response	Reference	Web link

<b>1,2 dichloropropane</b>	CAS 78-87-5	Assessor A:	D Brooks, Sirius	Assessor B:	J Lymer, Wardell Armstrong	Final review:	Panel/SF
		Date	14/04/2009	Date	13/03/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	Justification: Value chosen is only available data and is likely to be conservative
	38	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
WHO Guidelines for Drinking Water Quality	2003	Drinking water	38	ug day-1	Estimated maximum daily exposure for an adult consuming 2 litres of water per day	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/12dichloropropane/en/">http://www.who.int/water_sanitation_health/dwg/chemicals/12dichloropropane/en/</a>	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">www.who.int/water_sanitation_health/dwg/guidelines/en</a>

<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	Justification: Value chosen is only available data and is likely to be conservative
	5.2	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
WHO Guidelines for Drinking Water Quality	2003	Air concentration	5.2	ug day-1	Estimated exposure to 1,2-DCP based on average concentration measured in urban/suburban air in 1982 in Japan (0.26 ug/m <sup>3</sup> ) assuming an air intake of 20m <sup>3</sup> /day	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/12dichloropropane/en/">http://www.who.int/water_sanitation_health/dwg/chemicals/12dichloropropane/en/</a>	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">www.who.int/water_sanitation_health/dwg/guidelines/en</a>

Substance:	<b>1,2-Dichloropropane</b>	CAS Number:	78-87-5	Assessor A:	J Lymer / R Reuter, Wardell Armstrong	Assessor B:	D Brooks, Sirius	Final Review:	Panel/SF
Chemical Formula:	C <sub>3</sub> H <sub>5</sub> Cl <sub>2</sub>	Phase at Ambient Temperature	liquid	Date:	11-Mar-09	Date:	14-Apr-09	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oecd.org/scripts/hpv/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000									
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)				
<b>Required Parameters</b>																																					
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	<b>112.99</b>	n/a	Value from consistent range	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)							
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	<b>1.24E+02</b>	10	Measured value at temperature required for CLEA	Geomean	atm m <sup>3</sup> mol <sup>-1</sup>	Conservative value adopted	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)							
						2.07E-03	2.10E+02	25	ND	#VALUE!	25	2.98E+02	298	25	n/a	n/a	n/a	1.22E-03	123.6165	10	2.94E-03	297.8955	25	3.40E-01	2.95E+02	25	2.70E-03	273.5775	25	2.74E+02	25						
													31.21	31.21																							
													280	280																							
													210	210																							
													286	286																							
													362	362																							
													233	233																							
						Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	<b>2.05E+03</b>	10	No Consistent range at 10 degrees - use most recent source	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	
2.74E+03	2.74E+03	25	ND	#VALUE!	25							2.30E+03	2.30E+03	10	ND	#VALUE!	10	2.05E+03	2.05E+03	10	2.70E+03	2.70E+03	20	ND	#VALUE!	20	2.80E+03	2.80E+03	25								
Chemical Boiling Point (ambient pressure)	K	n/a	<b>3.70E+02</b>	n/a	Median value from consistent range	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)							
						96.37	369.52	n/a	96.4	369.55	n/a	96.4	369.55	n/a	95	368.15	n/a	96.22	369.37	n/a	96.4	369.55	n/a	370	370.00	n/a	96.4	369.55	n/a								
Chemical Melting Point (ambient pressure)	K	n/a	<b>1.73E+02</b>	n/a	Median value from consistent range	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)							
						-100.44	172.71	n/a	-100.4	172.75	n/a	-100.53	172.62	n/a	Insert Values	n/a	-100.4	172.75	n/a	-100.4	172.75	n/a	172.75	172.75	n/a	-100.4	172.75	n/a									
Log Octanol - Water Coefficient	Dimensionless	n/a	<b>1.99</b>	n/a	Medium confidence in central value from consistent range	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)							
						1.99	1.99	n/a	ND	ND	n/a	2	2.00	n/a	ND	ND	n/a	1.99	1.99	n/a	2.28	2.28	n/a	ND	ND	n/a	2	2.00	n/a								
						Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	<b>115.8</b>	n/a	Very low confidence / single reported value	Average	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	32283.17636	<b>3.23E+04</b>	Normal Chemical Boiling Point	Calculated value in agreement with measured values	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>		KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a								
						ND	#VALUE!	Normal Boiling Point	30.5	30500	Normal Boiling Point																										
						32.004	32004	Normal Boiling Point																													
Chemical Critical Point temperature (ambient pressure)	K	572.4097125	<b>572.4</b>	n/a	Calculated value in agreement with measured value	Average	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a									
						ND	ND	n/a	n/a	n/a	ND	#VALUE!	n/a	578	578.00	n/a	ND	#VALUE!	n/a																		
Critical Pressure	atm	41.80578495	<b>41.81</b>	n/a	Calculated value in agreement with measured value	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a									
						ND	#VALUE!	n/a	n/a	n/a	ND	#VALUE!	n/a	46.5	45.8919319	n/a	4.59E+01	n/a																			

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	7.193E-02	10	Estimated from parameters above using Clapryon relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	3072.314426	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	7.74E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	5.95E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	1.71	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Contaminant Name: 1,3,5 Trimethylbenzene	CAS Number: 108-67-8	Assessor A: Mathew Rouge	Assessor B: Gareth Wills	Final Review: Panel/SF
Date: Mar-09	Date: Apr-09	Date: 28/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDioral to exposure routes?	No	No	No	N/A	Insufficient data with sufficient detail in derivation to derive HCV. No information available regarding carcinogenicity
Apply IDoral to exposure routes?	No	No	No		
Apply TDinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	none	ug.kg-1.d-1	No recommended TDloral. Insufficient data with detail on derivation to derive TDloral

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2009	Jul-09	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Office of Environmental Health Hazard Assessment	<a href="http://oehha.ca.gov/water/pals/124135tmb.html">http://oehha.ca.gov/water/pals/124135tmb.html</a>	2001	Jul-09	RfD	47.66	ug/kg bw/day	47.66	Not provided	NOAEL	143	mg/kg-day	3000	10 for interspecies extrapolation, 10 for extrapolation from subchronic to chronic study, 10 for human variability, 3 for database deficiencies.	Subchronic rat study
Risk Assessment Information System	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>	2008	Mar-09	RfD	50	ug/kg bw/day	50	Low	NOAEL	Not provided	Not provided	3000	Not provided	Not provided
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>	2008	Mar-09	RfD	50	ug/kg bw/day	50	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided

TDI inhal	Recommended TDloral	Units	Justification
	none	ug.kg-1.d-1	No recommended TDlinh. Insufficient data with detail on derivation to derive TDlinhalation

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	2007	Mar-09	Workplace Exposure Limit	125 (All trimethylbenzene isomers)	mg/m3	35714.29 ug/kg bw/day	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2009	Jul-09	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Risk Assessment Information System	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>	2008	Mar-09	RfC	6.00E-03	mg/m3	1.71 ug/kg bw/d	low	NOAEL	18	mg/m3	3000	No details provided	Human study
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>	2008	Mar-09	RfC	6.00E-03	mg/m3	1.71 ug/kg bw/d	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided

ID oral	Recommended IDoral	Units	Justification
	none	ug.kg-1.d-1	No information available regarding carcinogenicity

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2009	Jul-09	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

ID inhal	Recommended IDinhal	Units	Justification
	none	ug.kg-1.d-1	No information available regarding carcinogenicity

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
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Contaminant Name: 1,3,5 Trimethylbenzene

TDI oral
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Organisation	Description	Target organ/Critical Effect	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	The database for 1,3,5-trimethylbenzene is inadequate to derive a provisional RfD	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>
Office of Environmental Health Hazard Assessment	Groups of 10 male and 10 female Sprague-Dawley rats were administered 1,3,5-TMB by gavage in corn oil.	Abnormal clinical observations consisted of discoloured and/or wet inguinal fur and salivation in the highest dose group of both sexes. Critical effects included increases in mean absolute liver weight and mean relative kidney weight.	IITRI (1995). 90-Day oral gavage toxicity study of 1,3,5-trimethylbenzene in rats with a recovery group. Industry Institute of Toxicology Research Institute. Study conducted for Koch Industries Inc., Wichita, KS.	<a href="http://oehha.ca.gov/water/pais/124135tmb.html">http://oehha.ca.gov/water/pais/124135tmb.html</a>
Risk Assessment Information System	Not provided	dec in body wt gain; clinical observations; inc liver/kidney wt in rats	IITRI (1995). 90-Day oral gavage toxicity study of 1,3,5-trimethylbenzene in rats with a recovery group. Industry Institute of Toxicology Research Institute. Study conducted for Koch Industries Inc., Wichita, KS.	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>
Texas Commission on Environmental Quality	The value is provided by the US EPA National Centre for Environmental Assessment (NCEA)	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>

TDI inhal
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Organisation	Description	Response	Reference	Web link
Health and Safety Executive (HSE)	8 hour long term workplace exposure limit	Not provided	Not provided	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Insufficient information to derive a provisional RfD for 1,3,5-trimethylbenzene. Battig study deemed to be insufficient. No chronic inhalation toxicity studies located.	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>
Risk Assessment Information System	Not provided	CNS effects, asthma-like bronchitis, anemia, blood clot effects	Battig et al 1958	<a href="http://rais.ornl.gov/tox/rap_toxp.shtml">http://rais.ornl.gov/tox/rap_toxp.shtml</a>
Texas Commission on Environmental Quality	The value is provided by the US EPA National Centre for Environmental Assessment (NCEA)	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>

ID oral
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Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	There are no human or animal carcinogenicity data	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>

ID inhal
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Organisation	Description	Response	Reference	Web link
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<b>1,3,5-Trimethylbenzene</b>	CAS 108-67-8	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
		Date	08/04/2009	Date	15/04/2009	Date	28/08/2009

MDI		Recommended MDIoral	Units	Justification: Only literature value obtained. Conservative, based on max recorded concentration in tap water (US National Tap Water Quality Database). Converted assuming 2L/day water consumed				
Organisation		Date	Media	Value	Units	Description	Reference	Web link
		8	ug day-1					
Other - National Tap Water Quality Database			tap water	max concentration in tap water 4ppb	8 ug/d (assuming 2litres of water/d)	value taken from highest recorded concentration in tap water, US. Converted to daily intake assuming 2 litres of water consumed per day.	National Tap Water Quality Database	<a href="http://www.ewg.org/tapwater/contaminants/contaminant.php?contamcode=2424">http://www.ewg.org/tapwater/contaminants/contaminant.php?contamcode=2424</a>

MDI		Recommended MDIinh	Units	Justification: only literature value obtained (TOXNET)				
Organisation		Date	Media	Value	Units	Description	Reference	Web link
		20.5	ug day-1					
Toxicological Data Network (TOXNET)		1985	Ambient Air	20.5	ug day-1	The average daily dose of 1,3,5-trimethylbenzene from breathing air in The Netherlands was estimated as 20.5 ug/day based on mean ambient air concentrations of 0.10-0.30 ppb ( conversion not detailed within Toxnet - but is assumed to be approximately 0.3e-9 x 1 atm x 120.19 g.mol-1 x 15 m3.d-1 x 1e6 ug.g-1 / ( 8.206e-5 atm.m3.mol-1.K-1 x 288 K)	Guicherit R, Schulting FL; Sci Total Environ 43: 193-219 (1985)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>



1-Methylnaphthalene	CAS Number:	90-12-0	Assessor A:	Andreas Neymeyer, Buro Happold	Assessor B:	Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF
	Date	16/04/2009	Date	16/04/2009	Date	28/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	NR	Chronic dietary studies with 1- or 2-methylnaphthalene provided limited evidence for carcinogenicity. Recommended IDoral is lower than TDloral, therefore IDoral adopted as oral HCV and applied to oral and dermal exposure.
Apply IDoral to exposure routes?	Yes	Yes	No		
Apply TDlinh to exposure routes?	No	No	No		No inhalation route health criteria value. Likely to be similar to naphthalene, i.e. inhalation orders of magnitude more toxic than oral
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	7	ug.kg-1.d-1	USEPA PPRTV concluded that there was insufficient data to derive a provisional RfD but derived a provisional toxicity screening value that may be of limited use to risk assessors. Despite these uncertainties, the facts that (1) the PPRTV report is more recent than the ATSDR report, (2) the PPRTV screening value is more conservative and (3) the PPRTV screening value is closer to the EIC proposed HCVoral for 2-methyl naphthalene, results in the PPRTV screening value being recommended as the TDloral.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Jul-09	15/07/2009	Provisional toxicity screening value	0.007	mg/kg/day	7		LOAEL	71.6	mg/kg body weight per day	10000	Composite uncertainty factor (UF) of 10,000, which includes factors of 10 for extrapolating from a LOAEL to a NOAEL, 10 for interspecies extrapolation, 10 for interindividual variability, and 10 for database deficiencies.	animal (mice)
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Aug-05	27/03/2009	MRL (substance-specific Minimal Risk Level)	0.07	mg/kg/day	70		LOAEL	71.6	mg/kg body weight per day	1000	10 for using a LOAEL, 10 for extrapolating from animals to humans, and 10 for human variability	animal (mice)

TDI inhal	Recommended TDlinhal	Units	Justification
	n/a		No inhalation route health criteria value. [The reasonable presumption of 1-methylnaphthalene to be similar to naphthalene (regarding its chemical and toxicological properties) would suggest risks from 1-methylnaphthalene to be dominated by the inhalation pathway. However, no human or animal data are available regarding the toxicity of 1-methylnaphthalene following repeated inhalation exposure.]

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>												No human or animal data are available regarding the toxicity of 1-methylnaphthalene following repeated inhalation exposure, thus precluding the derivation of provisional subchronic or chronic RfC values for 1-methylnaphthalene.	

ID oral	Recommended IDoral	Units	Justification
	2.3	ug.kg-1.d-1	Derived from BMDL10 for incidence of lung adenomas and carcinomas from Mutata et al 1993 study divided by uncertainty factor of 10,000, as recommended in Environment Agency SC050021/SR2 report, 2009

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Jan-08	15/07/2009	Cancer risk	Lung adenomas or carcinomas observed during 81-week mice study	Slope factor	0.029	(mg/kg/d) <sup>-1</sup>		Calculated based on a derived BMDL10 of 22.91 mg/kg/d	animal (mice)

ID inhal	Recommended IDinhal	Units	Justification
	n/a		Chronic dietary studies with 1- or 2-methylnaphthalene provided limited evidence for carcinogenicity.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>									There are no appropriate human or animal data from from which to derive an inhalation unit risk for 1-methylnaphthalene	

1-Methylnaphthalene

TDI oral

Organisation	Description	Target organ/Critical Effect	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	81-week oral study of male and female mice provide available carcinogenicity assay for 1-methylnaphthalene.  A chronic screening-value RfD of 7E-3 mg/kg-day based on pulmonary alveolar proteinosis in mice (Murata et al., 1993) is derived by dividing the LOAEL of 71.6 mg/kg-day by a composite uncertainty factor (UF) of 10,000, which includes factors of 10 for extrapolating from a LOAEL to a NOAEL, 10 for interspecies extrapolation, 10 for interindividual variability.	Pulmonary alveolar proteinosis in female mice	Appendix A of Superfund Health Risk Technical Support Center, National Center for Environmental Assessment, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH 45268 Provisional Peer Reviewed Toxicity Values for 1-Methylnaphthalene (CASRN 90-12-0)	<a href="http://www.epa.gov/iris">http://www.epa.gov/iris</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Chronic-duration study of 1-methylnaphthalene in the diet	Pulmonary alveolar proteinosis in female mice	Murata et al. 1993	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp67.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp67.pdf</a>

TDI inhal

Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				<a href="http://www.epa.gov/iris">http://www.epa.gov/iris</a>

ID oral

Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	81-week oral study of male and female mice provide available carcinogenicity assay for 1-methylnaphthalene (Mutata et al., 1993)	Increased incidences of lung adenomas or carcinomas (combined)	Superfund Health Risk Technical Support Center, National Center for Environmental Assessment, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, OH 45268 Provisional Peer Reviewed Toxicity Values for 1-Methylnaphthalene (CASRN 90-12-0)	<a href="http://www.epa.gov/iris">http://www.epa.gov/iris</a>

ID inhal

Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				<a href="http://www.epa.gov/iris">http://www.epa.gov/iris</a>

<b>1-Methylnaphthalene</b>	CAS 90-12-0	Assessor A:	Andreas Neymeyer, Buro Happold	Assessor B:	Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF
		Date	09/04/2009	Date	09/04/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> Exposure to methylnaphthalenes is mainly by inhalation.
	n/a		

Organisation	Date	Media	Value	Units	Description	Reference	Web link
<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Based on a single source of information available (ATSDR). Estimate is based on ambient air samples taken from 64 locations and assuming human daily intake of 20 m <sup>3</sup> .		
			10	ug day-1			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
<b>US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels</b>	27/03/2009	Air	10	ug day-1	Exposure to methylnaphthalenes is mainly by inhalation. The estimated average daily intake from ambient air may be about 10 µg. Estimate is based on ambient air samples taken from 64 locations and assuming human daily intake of 20 m <sup>3</sup>	Shah and Heyerdahl 1988 in Research Triangle Institute. 1995. TOXICOLOGICAL PROFILE FOR NAPHTHALENE, 1-METHYLNAPHTHALENE, AND 2-METHYLNAPHTHALENE. Prepared for: U.S. DEPARTMENT OF HEALTH AND HUMAN SERVICES Public Health Service Agency for Toxic Substances and Disease Registry ( <a href="http://72.30.186.56/search/cache?ei=UTF-8&amp;p=NAPHTHALENE%2C+1-METHYLNAPHTHALENE%2C+AND+2-METHYLNAPHTHALENE&amp;rd=r1&amp;fr=yfp-t-501&amp;u=www.regulations.gov/fdmspublic/ContentViewer%3FobjectId%3D09000064800c0b6d%26disposition%3Dattachment%26contentType%3Dpdf&amp;w=naphthalene+1+methylnaphthalene+2+methylnaphthalene&amp;d=MPzhTExISdsK&amp;icp=1&amp;.intl=uk">http://72.30.186.56/search/cache?ei=UTF-8&amp;p=NAPHTHALENE%2C+1-METHYLNAPHTHALENE%2C+AND+2-METHYLNAPHTHALENE&amp;rd=r1&amp;fr=yfp-t-501&amp;u=www.regulations.gov/fdmspublic/ContentViewer%3FobjectId%3D09000064800c0b6d%26disposition%3Dattachment%26contentType%3Dpdf&amp;w=naphthalene+1+methylnaphthalene+2+methylnaphthalene&amp;d=MPzhTExISdsK&amp;icp=1&amp;.intl=uk</a> )	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>

Substance:		1-Methylnaphthalene		CAS Number:		90-12-0		Assessor A:		Mike Rogers Andreas Neymeyer		Assessor B:		Andreas Neymeyer Mike Rogers		Final review:		Panel/SF												
Chemical Formula:		C11H10		Phase at Ambient Temperature:		Liquid		Date:		09/04/2009		Date:		16/04/2009		Date:		28/08/2009												
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000		
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	142.20	n/a	Little variation/consistently reported as 142.2g/mol	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	4.15E+01	25	No consistent range - most recent value	Geomean	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	2.05E+01	10	Solubility at assumed UK soil average temperature 10°C	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
Chemical Boiling Point (ambient pressure)	K	n/a	5.17E+02	n/a	Median value chosen as central value of consistent range	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Chemical Melting Point (ambient pressure)	K	n/a	2.47E+02	n/a	Median value chosen as central value of consistent range	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Log Octanol - Water Coefficient	Dimensionless	n/a	3.87	n/a	no consistent range - newest source (Montgomery, 2007) value chosen	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	1.70E+02	n/a	single literature value	Average	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	46208	4.62E+04	Normal Boiling Point	Calculated value chosen - this is similar to range of reported values	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
Chemical Critical Point temperature (ambient pressure)	K	760	760.3	n/a	Calculated value chosen - this is consistent to range of reported values	Average	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Critical Pressure	atm	32.0	32.03	?	Calculated value chosen - this is consistent to range of reported values	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	8.74E-03	10	Estimated from parameters above using Clapyron relationship or direct calculation
Vapour pressure at ambient soil temperature	Pa	2.97	10	Estimated from parameters above using Grain-Watson method
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	6.02E-06	10	Estimated from parameters above using Wilkie-Lee method
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	4.75E-10	10	Estimated from parameters above using Hayduk and Laudie method
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	3.23	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

<b>2,4-Dimethylphenol</b>	<b>CAS Number:</b>	<b>105-67-9</b>	<b>Assessor A:</b>	D Brooks, Sirius	<b>Assessor B:</b>	J Lymer, Wardell Armstrong	<b>Final Review:</b>	Panel/SF
	<b>Date</b>	01/04/2009	<b>Date</b>	14/04/2009	<b>Date</b>	28/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	Insufficient evaluation to determine with respect to a human carcinogen - TDloral applied to oral, dermal and inhalation routes  Inadequate data available to derive inhalation HCV
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

<b>TDI oral</b>	<b>Recommended TDloral</b>	<b>Units</b>	<b>Justification</b>
	20	ug.kg-1.d-1	Only available value from reliable source (IRIS) chosen

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/11/1990	13/03/2009	Oral Rfd	0.02	mg/kg/day	20	Medium-Low	NOAEL	50	mg/kg/day	3000	An uncertainty factor of 3000 was established: 10 each for inter- and intraspecies variability and 30 for lack of chronic toxicity data, data in a second species and reproductive/developmental studies
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	27/06/2007	15/07/2009	Subchronic Oral Rfd	0.05	mg/kg/day	50		NOAEL	50	mg/kg/day	1000	10 for interspecies; 10 for intraspecies; 10 for database insufficiencies

<b>TDI inhal</b>	<b>Recommended TDlinhal</b>	<b>Units</b>	<b>Justification</b>
	N/A		Inadequate data available to derive inhalation HCV

Organisation	Last Updated	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
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<b>ID oral</b>	<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
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<b>ID inhal</b>	<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
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**2,4-Dimethylphenol**


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**TDI oral**


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Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	Mouse subchronic oral gavage	2,4-Dimethylphenol was administered daily to male and female albino mice by gavage for 90 days.	Clinical signs (lethargy, prostration, and ataxia) and haematological changes	U.S. EPA. 1989. Ninety-day gavage study in Albino mice using 2,4-dimethylphenol. Study No. 410-2831, prepared by Dynamac Corporation, Rockville, MD, for the Office of Solid Waste and Emergency Response, Washington, DC	<a href="http://www.epa.gov/ncea/iris/subst/0466.htm#reforal">http://www.epa.gov/ncea/iris/subst/0466.htm#reforal</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Mouse subchronic oral gavage	2,4-Dimethylphenol was administered daily to male and female albino mice by gavage for 90 days.	Clinical signs (lethargy, prostration, and ataxia) and hematological changes	U.S. EPA. 1989. Ninety-day gavage study in Albino mice using 2,4-dimethylphenol. Study No. 410-2831, prepared by Dynamac Corporation, Rockville, MD, for the Office of Solid Waste and Emergency Response, Washington, DC	

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**TDI inhal**


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Organisation	Study type	Description	Response	Reference	Web link
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**ID oral**


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Organisation	Study type	Description	Response	Reference	Web link
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**ID inhal**


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Organisation	Study type	Description	Response	Reference	Web link
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<b>2,4-Dimethylphenol</b>	<b>CAS 105-67-9</b>	Assessor A:	D Brooks, Sirius	Assessor B:	J Lymer, Wardell Armstrong	Final Review:	Panel/SF
		Date	01/04/2009	Date	14/04/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, likely to be negligible. HCV is equivalent to drinking water concentration of 700µg/L (based on a 70kg adult consuming 2L/day). This is significantly greater than analytical detection limit, so can assume that if not detected in majority of drinking water supplies, can assume negligible intake from water.
	0	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> No data, likely to be negligible.
	0	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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<b>2,4-Dinitrotoluene</b>	<b>CAS Number:</b>	<b>121-14-2</b>	<b>Assessor A:</b>	J Lymer, Wardell Armstrong	<b>Assessor B:</b>	D Brooks, Sirius	<b>Final review:</b>	Panel/SF
			<b>Date</b>	13/03/2009	<b>Date</b>	14/04/2009	<b>Date</b>	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	No	Group 2B carcinogen (IARC), possibly carcinogenic to humans. No health criteria available for non-threshold effects therefore HCV based on derived TDI. TDloral applied to oral,dermal and inhalation routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral				Recommended TDloral	Units	Justification
				2	µg/kg/day	Conservative value adopted, reported by three reliable sources (ATSDR, US EPA Health Advisors, IRIS)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Feb-08	13/03/2009	No health criteria value	N/A	N/A	N/A	N/A	LOAEL	0.57	mg/kg/day	N/A	N/A	24 month rat study
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	14/08/1997	13/03/2009	No health criteria value										
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	<a href="http://inchem.org/pages/sids.html">http://inchem.org/pages/sids.html</a>	Nov-97	13/03/2009	No health criteria value				N/A	NOEL	0.57-0.71	mg/kg/day	None		It is mutagenic in the Ames test and in in vivo tests on mammals.
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Original December 1998 and published as MRL December 2008	13/03/2009	Chronic Oral MRL	0.002	mg/kg/day	2	N/A	NOAEL	0.2	mg/kg/day	100	uncertainty factor of 100 (10 for animal-to-human extrapolation and 10 for human variability).	Dog Feeding Study 2-Year - neurotoxicity
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	01/01/2008 and August 2006	13/03/2009	Oral RfD	0.002	mg/kg/day	2	N/A	NOAEL	0.2	mg/kg/day	100	This uncertainty factor includes a factor of 10 for interspecies variability and a factor of 10 for intraspecies variability	Dog Feeding Study 2-Year - neurotoxicity
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/02/1993	13/03/2009	Oral RfD	0.002	mg/kg/day	2	High to medium	NOAEL	0.2	mg/kg/day	100	This uncertainty factor includes a factor of 10 for interspecies variability and a factor of 10 for intraspecies variability	Dog Feeding Study 2-Year - neurotoxicity

TDI inhal				Recommended TDlinh	Units	Justification
						Inadequate data available to derive inhalation HCV

Organisation	Last Updated	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
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ID oral				Recommended IDoral	Units	Justification

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
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ID inhal				Recommended IDinhal	Units	Justification

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
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**2,4-Dinitrotoluene**

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
European Chemicals Bureau (ECB)	N/A	the critical effects for risk characterisation derived from the 24-month rat study were presence of hyperplastic foci in the liver and atrophy of seminiferous tubules.	European Union Risk Assessment Report 2,4-dinitrotoluene	ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/24dinitrotoluenereport411.pdf
International Agency for Research on Cancer (IARC)	2,4- and 2,6-Dinitrotoluenes are possibly carcinogenic to humans (Group 2B).			<a href="http://www.inchem.org/documents/iarc/vol65/dinitrotoluene.html">http://www.inchem.org/documents/iarc/vol65/dinitrotoluene.html</a>
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals		No teratogenic effects were recorded and impairment of fertility were observed at doses which also cause other effects.	2,4-Dinitrotoluene	<a href="http://inchem.org/documents/sids/sids/121142.html">http://inchem.org/documents/sids/sids/121142.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Beagle dogs were administered 0,0.2, 1.5, or 10 mg.kg 2,4-DNT in capsules for up to 24 months.	Methemoglobinemia and Heinz bodies were observed in dogs fed 1.5 mg/kg. Biliary hyperplasia and neurotoxicity (paralysis and cerebellar lesions) were also noted at this dose. No testicular degeneration was observed up to 10 mg.kg 2,4-DNT	Toxicological Profile for 2,4- and 2,6-Dinitrotoluene December 1998 and ATSDR Minimal Risk Levels (MRLs) December 2008	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp109.html">http://www.atsdr.cdc.gov/toxprofiles/tp109.html</a> <a href="http://www.atsdr.cdc.gov/mrls/">http://www.atsdr.cdc.gov/mrls/</a>
USEPA Health Advisors	Groups of beagle dogs (6/sex/dose) were fed 2,4-DNT in gelatin capsules at 0, 0.2, 1.5, or 10 mg/kg/day.	Neurotoxicity, Heinz bodies and biliary tract hyperplasia	Drinking Water Health Advisories 2006 Edition and Drinking Water Health Advisory for 2,4-Dinitrotoluene and 2,6-Dinitrotoluene	<a href="http://www.epa.gov/waterscience/criteria/drinking/dwstandards">http://www.epa.gov/waterscience/criteria/drinking/dwstandards</a> <a href="http://www.epa.gov/safewatr/ccl/pdf/DNTs.pdf">www.epa.gov/safewatr/ccl/pdf/DNTs.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Groups of beagle dogs (6/sex/dose) were fed 2,4-DNT in gelatin capsules at 0, 0.2, 1.5, or 10 mg/kg/day.	Neurotoxicity, Heinz bodies and biliary tract hyperplasia	IRIS 2,4-Dinitrotoluene	<a href="http://www.epa.gov/ncea/iris/subst/0524.htm">http://www.epa.gov/ncea/iris/subst/0524.htm</a>
TDI inhal				
Organisation	Description	Response	Reference	Web link
ID oral				
Organisation	Description	Response	Reference	Web link
ID inhal				
Organisation	Description	Response	Reference	Web link

<b>2,4-Dinitrotoluene</b>	CAS 121-14-2	Assessor A:	J Lymer, Wardell Armstrong	Assessor B:	D, Brooks, Sirius	Final review:	Panel/SF
		Date	13/03/2009	Date	14/04/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification: No data, background exposure assumed negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 70µg/L based on a 70kg adult consuming 2L/day.</b>
	0	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification: No data, likely to be negligible</b>		
			0	ug day <sup>-1</sup>			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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Substance:	<b>2,4-Dinitrotoluene</b>	CAS Number:	121-14-2	Assessor A:	J Lymer / R Reuter, Wardell Armstrong	Assessor B:	D Brooks, Sirius	Final review:	Panel/SF
Chemical Formula:	C <sub>7</sub> H <sub>5</sub> N <sub>2</sub> O <sub>4</sub>	Phase at Ambient Temperature	Solid	Date:	11/03/2009	Date:	14/04/2009	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>

<http://webbook.nist.gov/chemistry/>

<http://cs3-hq.oecd.org/scripts/hqv/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000									
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)				
<b>Required Parameters</b>																																					
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	182.134	n/a	Median value from consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)							
						Average	182.13	182.13	n/a	182.14	182.14	n/a	182.134	182.134	n/a	Insert Values	n/a	182.14	182.14	n/a	Insert Values	n/a	182.1336	182.1336	n/a	182.1336	182.1336	n/a	Insert Values	n/a							
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	5.46E-03	25	Newest reported value as no consistent range		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)							
						Geomean	8.67E-07	8.78E-02	25	ND	#VALUE!	25	1.60E-02	0.016	0.456	0.456	0.0878	0.0878	32.23	32.23	25	n/a	n/a	n/a	5.39E-08	0.005461418	25	ND	#VALUE!	25	2.10E+01	4.78E+00	25	ND	#VALUE!	25	
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	1.29E+02	12.4	Reported value measured at 12.4 degrees, the closest temperature to CLEA input		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)				
						Geomean	3.00E+02	3.00E+02	ND	#VALUE!	2.76E+02	2.76E+02	ND	#VALUE!	2.76E+02	2.76E+02	ND	#VALUE!	1.29E+02	1.29E+02	12.4	ND	#VALUE!	ND	#VALUE!	ND	#VALUE!	ND	#VALUE!	ND	#VALUE!	ND	#VALUE!	ND	#VALUE!		
Chemical Boiling Point (ambient pressure)	K	n/a	573.15	n/a	Consistent values - potential for decomposition noted		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	K	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)				
						Average	300	573.15	n/a	300	573.15	n/a	300	573.15	n/a	Insert Values	n/a	300	573.15	n/a	Insert Values	n/a	300	573.15	n/a	300	573.15	n/a	Insert Values	n/a	300	573.15	n/a	Insert Values	n/a		
Chemical Melting Point (ambient pressure)	K	n/a	344.15	n/a	Median value from consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	K	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)				
						Average	71	344.15	n/a	71	344.15	n/a	70.5	343.65	n/a	Insert Values	n/a	71.1	344.25	n/a	Insert Values	n/a	71	344.25	n/a	341	341.00	n/a	343	343.00	n/a	345	345.00	n/a	343	343.00	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	1.98	n/a	Median value from consistent range		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)				
						Average	1.98	1.98	n/a	ND	ND	n/a	1.98	1.98	n/a	ND	ND	n/a	1.98	1.98	n/a	ND	ND	n/a	ND	ND	n/a	ND	ND	n/a	ND	ND	n/a	ND	ND		
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	175.2	n/a	Single reported value		n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
						Average	n/a	n/a	n/a	n/a	n/a	n/a	175.2	175.20	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	60965.08192	6.10E+04	Normal Boiling Point	Calculated Value		n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
						Average	n/a	n/a	n/a	33.2	33200	Normal Boiling Point	ND	#VALUE!	Normal Boiling Point	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
Chemical Critical Point temperature (ambient pressure)	K	791.0055977	791.0	n/a	Calculated Value		n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
						Average	n/a	n/a	n/a	ND	ND	n/a	n/a	n/a	n/a	ND	#VALUE!	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
Critical Pressure	atm	33.51945437	33.52	n/a	Calculated Value		n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			
						Average	n/a	n/a	n/a	ND	#VALUE!	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a			

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	3.672E-07	10	Estimated from parameters above using Claypyron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	0.015351668	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	5.71E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	4.66E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	2.15	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

<b>2,6-Dinitrotoluene</b>	<b>CAS Number:</b>	<b>606-20-2</b>	Assessor A: D Brooks, Sirius	Assessor B: J Lymer, Wardell Armstrong	Final review: Panel/SF	
	Date	13/03/2009	Date	14/04/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	Group 2B carcinogen (IARC), possibly carcinogenic to humans. No health criteria available for non-threshold effects therefore HCV based on derived TDI. TDloral applied to oral,dermal and inhalation routes  Inadequate data available to derive inhalation HCV
Apply IDoral to exposoure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

<b>TDI oral</b>	<b>Recommended TDloral</b>	<b>Units</b>	<b>Justification</b>
	1	µg/kg/day	Only available value from reliable sources (USEPA Health Advisors and USEPA PPRTV) chosen

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Agency for Research on Cancer (IARC)	<a href="http://incem.org/pages/iarc.html">http://incem.org/pages/iarc.html</a>	14/08/1997	13/03/2009	No health criteria value									
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Original December 1998 and published as MRL December 2008	13/03/2009	No health criteria value									
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/dinking">http://www.epa.gov/waterscience/criteria/dinking</a>	01/01/2008 and August 2006	13/03/2009	Oral Rfd	0.001	mg/kg/day	1	N/A	NOAEL	4	mg/kg/day	3000	Includes a tenfold UF for intraspecies variability, another tenfold UF to account for interspecies extrapolation, and another tenfold UF for use of a less-than-lifetime study. An additional factor of 3 is used to account for the limited database.
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtm">http://rais.ornl.gov/tox/unauthorized.shtm</a>	13/12/2004	15/07/2009	Chronic Rfd	0.001	mg/kg/day	1	N/A	NOAEL	4	mg/kg/day	3000	10 for interspecies; 10 for intraspecies; 3 for database limitations & 10 for subchronic to chronic

<b>TDI inhal</b>	<b>Recommended TDlinh</b>	<b>Units</b>	<b>Justification</b>
	N/A		Inadequate data available to derive inhalation HCV

Organisation	Last Updated	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
<b>ID oral</b>											

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
<b>ID inhal</b>								

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis

**2,6-Dinitrotoluene**

**TDI oral**

Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
International Agency for Research on Cancer (IARC)		2,4- and 2,6-Dinitrotoluenes are possibly carcinogenic to humans (Group 2B).			
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels				Toxicological Profile for 2,4- and 2,6-Dinitrotoluene December 1998 and ATSDR Minimal Risk Levels (MRLs) December 2008	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp109.html">http://www.atsdr.cdc.gov/toxprofiles/tp109.html</a> <a href="http://www.atsdr.cdc.gov/mrls/">http://www.atsdr.cdc.gov/mrls/</a>
USEPA Health Advisors	Dog Feeding 13-week study	The dogs (4/sex/dose) were given 2,6-DNT in capsules at doses of 0, 4, 20, or 100 mg/kg/day for 13 weeks. There were no adverse effects observed in the low-dose animals. 2,6-DNT did, however, produce toxicity at higher dose levels	The animals had BW loss due to decreased food consumption. Adverse effects in this study were neurological and hematological, and there were altered clinical chemistry parameters. There also were bile duct hyperplasia and histopathological effects to the liver and kidneys of both sexes and to the testes in males.	Drinking Water Health Advisories 2006 Edition and Drinking Water Health Advisory for 2,4-Dinitrotoluene and 2,6-Dinitrotoluene	<a href="http://www.epa.gov/waterscience/criteria/drinking/dwstandards_www.epa.gov/safewatr/ccl/pdf/DNTs.pdf">http://www.epa.gov/waterscience/criteria/drinking/dwstandards_www.epa.gov/safewatr/ccl/pdf/DNTs.pdf</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Dog Feeding 13-week study	The dogs (4/sex/dose) were given 2,6-DNT in capsules at doses of 0, 4, 20, or 100 mg/kg/day for 13 weeks. There were no adverse effects observed in the low-dose animals. 2,6-DNT did, however, produce toxicity at higher dose levels	The animals had BW loss due to decreased food consumption. Adverse effects in this study were neurological and hematological, and there were altered clinical chemistry parameters. There also were bile duct hyperplasia and histopathological effects to the liver and kidneys of both sexes and to the testes in males.	Lee, C-C., H.V. Ellis, J.J. Kowalski et al. 1976. Mammalian toxicity of munition compounds Phase II: Effects of multiple doses. Part III: 2,6-Dinitrotoluene. Study conducted by the Midwest Research Institute for the U.S. Medical Bioengineering Research and Development Laboratory. Fort Detrick, Frederick, MD. AD A 062 015.	

**TDI inhal**

Organisation	Study type	Description	Response	Reference	Web link
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**ID oral**

Organisation	Study type	Description	Response	Reference	Web link
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**ID inhal**

Organisation	Study type	Description	Response	Reference	Web link
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<b>2,6-Dinitrotoluene</b>	CAS 606-20-2	Assessor A:	D, Brooks, Sirius	Assessor B:	J Lymer, Wardell Armstrong	Final review:	Panel/SF
		Date	13/03/2009	Date	14/04/2009	Date	28/08/2009

MDI	Recommended MDI <sub>oral</sub>	Units	Justification: No data, background exposure assumed negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 35µg/L based on a 70kg adult consuming 2L/day.
	0	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
MDI			Recommended MDI <sub>inh</sub>	Units	Justification: No data, likely to be negligible		
			0	ug day <sup>-1</sup>			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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Substance:	2,6-Dinitrotoluene	CAS Number:	606-20-2	Assessor A:	D Brooks, Sirius	Assessor B:	J Lymer / R Reuter, Wardell Armstrong	Final review:	Panel/SF
Chemical Formula:	C <sub>7</sub> H <sub>5</sub> N <sub>2</sub> O <sub>4</sub>	Phase at Ambient Temperature	Solid	Date:	11/03/2009	Date:	14/04/2009	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>

<http://webbook.nist.gov/chemistry/>

<http://cs3-hq.oecd.org/scripts/hpy/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000		
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	182.13	n/a	Value from consistent range	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	2.20E-02	25	Newest reported value used as no consistent range	Geomean	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	2.32E+02	25	Newest reported value used as no consistent range	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
Chemical Boiling Point (ambient pressure)	K	n/a	558.2	n/a	Same values	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Chemical Melting Point (ambient pressure)	K	n/a	339.15	n/a	Median value from consistent range	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Log Octanol - Water Coefficient	Dimensionless	n/a	2.10	n/a	Newest reported value as no consistent range	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	175.2	n/a	Single reported value	Average	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	59370.30343	5.94E+04	n/a	Normal Chemical Boiling Point	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Chemical Critical Point temperature (ambient pressure)	K	770.3040641	770.3	n/a	Calculated Value	Average	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Critical Pressure	atm	33.51945437	33.52	n/a	Calculated Value	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Recommended Literature Value	Rationale	Property	Units	Calculated Value	Recommended Literature Value	Rationale	Property	Units	Calculated Value	Recommended Literature Value	Rationale	Property	Units	Calculated Value	Recommended Literature Value	Rationale					
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	1.569E-06	n/a	Estimated from parameters above using Clapron relationship or direct calculation	Vapour pressure at ambient soil temperature	Pa	0.037153137	n/a	Estimated from parameters above using Grain-Watson method	Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	5.74E-06	n/a	Estimated from parameters above using Wilkie-Lee method	Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	4.66E-10	n/a	Estimated from parameters above using Hayduk and Laudie method	Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	2.22	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

2-chloronaphthalene	CAS Number:	91-58-7	Assessor A:	Y Macklin, AMEC	Assessor B:	K Privett, Hydrock	Final review:	Panel/SF
	Date	25/03/2009	Date	08/05/2009	Date	26/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Not evaluated for human carcinogenicity (IRIS).
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		Not evaluated for human carcinogenicity (IRIS).

TDI oral	Recommended TDloral	Units	Justification
	80	ug.kg-1.d-1	Consensus between IRIS and RIVM.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg.1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	unknown	08/04/2009	Concludes that there is not sufficient information to derive NOAEL or LOAEL										
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	unknown	08/04/2009	TDI (chloronaphthalenes-SUM)	80	ug/kg bw/day	80	Low	NOAEL	250	mg/kg bw/day	3000	An uncertainty factor of 3000 reflects 10 each for inter- and intraspecies conversion, 10 for the use of a subchronic study for chronic RfD derivation, and 3 to account for the lack of reproductive/developmental and chronic toxicity data.	Mouse Subchronic Oral Gavage Study.
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	23/01/2008	08/04/2009	RfD for beta-chloronaphthalene	8.00E-02	mg/kg bw/day	80	Low/medium	LOAEL NOAEL	600 250	mg/kg/day mg/kg/day	3000	An uncertainty factor of 3000 reflects 10 each for inter- and intraspecies conversion, 10 for the use of a subchronic study for chronic RfD derivation, and 3 to account for the lack of reproductive/developmental and chronic toxicity data.	Mouse Subchronic Oral Gavage Study.
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	unknown	08/04/2009	RfD	8.00E-02	mg/kg bw/day	80		LOAEL NOAEL	600 250	mg/kg/day mg/kg/day	3000	An uncertainty factor of 3000 reflects 10 each for inter- and intraspecies conversion, 10 for the use of a subchronic study for chronic RfD derivation, and 3 to account for the lack of reproductive/developmental and chronic toxicity data.	

TDI inhal	Recommended TDlinhal	Units	Justification
	0.286	ug.kg-1.d-1	In the absence of any other data the provisional Dutch RIVM value has been adopted.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg.1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	unknown	08/04/2009	provisional TCA	1	ug/m3	0.286	Low	NOAEC	1.3	mg/m3	900	3 x for extrapolation of LOAEC to NOAEC. An additional UK of 100 for inter- and intraspecies variation. And a further factor of 3 is used to correct for the restricted database. With a correction factor of 0.7 for continuous exposure.	

ID oral	Recommended IDoral	Units	Justification
	n/a		This substance/agent has not undergone a complete evaluation and determination under US EPA's IRIS program for evidence of human carcinogenic potential.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
ID inhal	Recommended IDinhal	Units	Justification								
	n/a		This substance/agent has not undergone a complete evaluation and determination under US EPA's IRIS program for evidence of human carcinogenic potential.								

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type

2-chloronaphthalene

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)			CICAD 34 (2001) Chlorinated Naphthalenes	<a href="http://www.inchem.org/documents/cicads/cicads/cicad34.htm">http://www.inchem.org/documents/cicads/cicads/cicad34.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	13 week study in mice (see detailed description below).	Liver	US EPA study (see below)	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701023.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701023.pdf</a> <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
USEPA Integrated Risk Information System (IRIS)	CD-1 mice (20/sex/group) were administered oral gavage dosages of 0, 100, 250, or 600 mg/kg/day beta-chloronaphthalene in corn oil for 13 weeks. Parameters examined included mortality, body and organ weight changes, food consumption, clinical signs, ophthalmologic changes, haematology, clinical chemistry, and gross histopathology. The LOAEL was identified as 600 mg/kg/day and the NOAEL was 250 mg/kg/day.	Dyspnea, abnormal appearance, liver enlargement	U.S. EPA. 1989. Subchronic study in mice with beta-Chloronaphthalene. HLA Study No. 2399-124. Prepared by Hazleton Laboratories America, Inc. for U.S. EPA, Office of Solid Waste, Washington, DC.	<a href="http://www.epa.gov/ncea/iris/subst/0463.htm">http://www.epa.gov/ncea/iris/subst/0463.htm</a>
Toxicology Data Network (Toxnet)	As per USEPA study	USEPA study above	USEPA study above	USEPA study above
TDI inhal				
Organisation	Description	Response	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Rats exposed for a period of 134 days, 16 hours per day.	Liver	TSD (1993) Environmental Hazard Assessment: halogenated naphthalenes. Toxic Substances Division, Dir. Air, Climate and Toxic Substances. Building Res. Establishment, Garston, Watford UK.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701023.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701023.pdf</a> <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
ID oral				
Organisation	Description	Response	Reference	Web link
ID inhal				
Organisation	Description	Response	Reference	Web link

2-chloronaphthalene	CAS 91-58-7	Assessor A:	Y Macklin, AMEC	Assessor B:	K Privett, Hydrock	Final review:	Panel/SF
		Date	25/03/2009	Date	08/05/2009	Date	26/08/2009

MDI	Recommended MDI <sub>oral</sub>	Units	Justification: value for Netherlands in drinking water is used as considered most relevant to UK. Contribution from dietary sources is negligible.
	0.0001	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	08/04/2009	Drinking water	0.00088	ng/l	Study on levels of mono and dichloronaphthalene in drinking water in Japan. After chlorination, levels of 0.03–0.44 ng/litre for chloronaphthalene and levels of not detected to 0.15 ng/litre for dichloronaphthalene. Multiply by 2l per day for adult consumption. Convert from ng/l to µg/l divide by 1,000.	Shiraishi H, Pilkington NH, Otsuki A, Fuwa K (1985) Occurrence of chlorinated polynuclear aromatic compounds in tap water. Environmental science and technology, 19:585–590.	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	08/04/2009	Drinking water and food	0.0001	µg/day	Chloronaphthalene can be found in drinking water after chlorination processing, leading to a daily intake in the order of 0.1 ng. The exposure of the population from 1- and 2-chloronaphthalene from food is negligible. Convert from ng/l to µg/l divide by 1,000.	TSD (1993) Environmental Hazard Assessment: halogenated naphthalenes. Toxic Substances Division, Dir. Air, Climate and Toxic Substances. Building Res. Establishment, Garston, Watford UK. ( <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> )	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
MDI			Recommended MDI <sub>inh</sub>	Units	Justification: Netherlands value used as study is likely to be more relevant to the UK.		
			0.02	ug day-1			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	08/04/2009	Ambient air	0.003	µg day-1	Chlorinated naphthalene concentrations of up to 150 pg/m <sup>3</sup> at "semi rural" sites and 1–40 pg/m <sup>3</sup> at remote sites. Conversion from original data: multiply by 20m <sup>3</sup> to allow for adult inhalation according EA toxicological guidance. Convert from pg/day to µg/day divide by 1,000,000.	<a href="http://www.inchem.org/documents/cicads/cicads/cicad34.htm">http://www.inchem.org/documents/cicads/cicads/cicad34.htm</a>	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	08/04/2009	Ambient air	0.02	µg day-1	According to TSD (1993) the lower chlorinated naphthalenes can be found in ambient air in the neighbourhood if different sources, from these data a concentration in the order of 1 ng/m <sup>3</sup> can be estimated in residential areas. Conversion from original data: multiply by 20m <sup>3</sup> . Convert from ng/day to µg/day divide by 1,000.	TSD (1993) Environmental Hazard Assessment: halogenated naphthalenes. Toxic Substances Division, Dir. Air, Climate and Toxic Substances. Building Res. Establishment, Garston, Watford UK. ( <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> )	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>

Substance:		2-Chloronaphthalene		CAS Number:	91-58-7	Assessor A:	K Privett, Hydrock	Assessor B:	Y Macklin, Amec	Final review:	Panel/SF																			
Chemical Formula:		C10H7Cl		Phase at Ambient Temperature:	Solid	Date:	16/03/2009	Date:	08/05/2009	Date:	26/08/2009																			
										<a href="http://srdata.nist.gov/solubility/">http://srdata.nist.gov/solubility/</a> <a href="http://webbook.nist.gov/chemistry/">http://webbook.nist.gov/chemistry/</a> <a href="http://cs3-hq.oesd.org/scripts/hpy/">http://cs3-hq.oesd.org/scripts/hpy/</a>																				
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al. 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000		
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	162.62	n/a	Consensus		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
							no data	#VALUE!	n/a	162.616	162.616	n/a	162.616	162.616	n/a	162.62	162.62	n/a	162.62	162.62	n/a	no data	#VALUE!	n/a	162.6153	162.6153	n/a	no data	#VALUE!	n/a
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	33.5	25	No consistent range - median value from most recent review chosen (Lide 2008)		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
							no data	#VALUE!	n/a	0.0335	3.35E+01	25	31.9	31.9	25	n/a	n/a	n/a	3.31E-04	33.538575	25	no data	#VALUE!	n/a	3.1	3.24E+01	25	no data	#VALUE!	n/a
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	11.7	25	No consistent range - median value from most recent review chosen (Lide 2008)		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
							no data	#VALUE!	n/a	1.17E-02	1.17E+01	25	11.7	1.17E+01	25	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Chemical Boiling Point (ambient pressure)	K	n/a	529	n/a	Consensus		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							no data	#VALUE!	n/a	256	529.15	n/a	256	529.15	n/a	256	529.15	n/a	256	529.15	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Chemical Melting Point (ambient pressure)	K	n/a	331	n/a	Consensus		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							no data	#VALUE!	n/a	58	331.15	n/a	58	331.15	n/a	59.5	332.65	n/a	58	331.15	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	3.98	n/a	Value from most recent study as only 2 values		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
							no data	#VALUE!	n/a	3.98	3.98	n/a	4.8	4.80	n/a	no data	#VALUE!	n/a	3.91	3.91	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	169	n/a	Single value		n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
													168.5	168.50	n/a															
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	47718.68387	4.77E+04	n/a	Normal Chemical Boiling Point		n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
							no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Chemical Critical Point temperature (ambient pressure)	K	780.6057495	780.6	n/a	Calculated value as no data		n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
							no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Critical Pressure	atm	33.59917355	33.60	n/a	Calculated value as no data		n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	3.78E-03	10	Estimated from parameters above using Claryon relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	0.501	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	5.95E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	4.77E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	3.32	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

2-Methylnaphthalene	CAS Number:	91-57-6	Assessor A: Andreas Neymeyer, Buro Happold	Assessor B: Mike Rogers, OPUS JOYNES PIKE Ltd	Final review: Panel/SF
			Date: 16/04/2009	Date: 16/04/2009	Date: 28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	NR	Chronic dietary studies with 1- or 2-methylnaphthalene provided limited evidence for carcinogenicity.  No inhalation route health criteria value. Likely to be similar to naphthalene, i.e. inhalation orders of magnitude more toxic than oral
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	4	ug.kg <sup>-1</sup> .d <sup>-1</sup>	Lowest literature oral Reference Dose (RfD) [USEPA Integrated Risk Information System (IRIS)]

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg <sup>-1</sup> .d <sup>-1</sup>	Confidence rating	Basis	Value	Units	UF	UF description	Study type
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	09/03/2009	27/03/2009	MRL (substance-specific Minimal Risk Level)	0.04	mg/kg/day	40		LOAEL BMDL05	50.3	mg/kg body weight per day	100	Based on the lower 95% confidence limit on a benchmark dose associated with 5% extra risk (BMDL05=4 mg/kg/day) for pulmonary alveolar proteinosis in male mice exposed to 2-methylnaphthalene in the diet for 81 weeks and an uncertainty factor of 100 (10 for extrapolation from animals to humans and 10 for human variability)	animal (mice)
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	09/03/2009	27/03/2009	RfD	0.004	mg/kg/day	4		BMDL05	3.5	mg/kg body weight per day	1000	A total uncertainty factor of 1000 was applied to the BMDL05 of 3.5 mg/kg-day: 10 for extrapolation for interspecies differences (UFA: animal to human); 10 for consideration of intraspecies variation (UFH: human variability); and 10 for deficiencies in the database (UFD).	animal (mice)
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Sep-07	15/07/2009	p-RfD	0.004	mg/kg/day	4		BMDL05	3.5	mg/kg body weight per day	1000	A total UF of 1000 was applied to this effect level: 10 for interspecies differences (UFA: animal to human); 10 for intraspecies variation (UFH: human variability); and 10 for deficiencies in the database (UFD).	animal (mice)

TDI inhal	Recommended TDlinhal	Units	Justification
	n/a		Insufficient data for the assessment of chronic risk to humans

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg <sup>-1</sup> .d <sup>-1</sup>	Confidence rating	Basis	Value	Units	UF	UF description	Study type
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>								Insufficient data for the assessment of chronic risk to humans with respect to the inhalation pathway					
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>								A provisional inhalation RfC could not be derived for 2-MN because data on adverse health effects following inhalation exposure were lacking for humans and animals.					

ID oral	Recommended IDoral	Units	Justification
	n/a		Chronic dietary studies with 1- or 2-methylnaphthalene provided limited evidence for carcinogenicity.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>				Quantitative estimates of cancer risk for 2-MN could not be derived because no data demonstrating carcinogenicity associated with 2-MN exposure were identified.						

ID inhal	Recommended IDinhal	Units	Justification
	n/a		Chronic dietary studies with 1- or 2-methylnaphthalene provided limited evidence for carcinogenicity.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>				Quantitative estimates of cancer risk for 2-MN could not be derived because no data demonstrating carcinogenicity associated with 2-MN exposure were identified.						

2-Methylnaphthalene

TDI oral
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Organisation	Description	Target organ/Critical Effect	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Chronic-duration study of 2-methylnaphthalene in the diet	Pulmonary alveolar proteinosis in female mice	Murata et al. 1993	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp67.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp67.pdf</a>
USEPA Integrated Risk Information System (IRIS)			Murata et al. 1997	<a href="http://www.epa.gov/iris/subst/1006.htm">http://www.epa.gov/iris/subst/1006.htm</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)			Murata et al. 1997	<a href="http://www.epa.gov/iris">http://www.epa.gov/iris</a>

TDI inhal
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Organisation	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)				<a href="http://www.epa.gov/iris/subst/1006.htm">http://www.epa.gov/iris/subst/1006.htm</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				<a href="http://www.epa.gov/iris">http://www.epa.gov/iris</a>

ID oral
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Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				

ID inhal
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Organisation	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				

<b>2-Methylnaphthalene</b>	CAS 91-57-6	Assessor A:	Andreas Neymeyer, Buro Happold	Assessor B:	Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF
		Date:	09/04/2009	Date:	09/04/2009	Date:	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> Exposure to methylnaphthalenes is mainly by inhalation.
	n/a		

Organisation	Date	Media	Value	Units	Description	Reference	Web link
<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Based on a single source of information available (ATSDR). Estimate is based on ambient air samples taken from 64 locations and assuming human daily intake of 20 m <sup>3</sup> .		
			1	ug day <sup>-1</sup>			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
<b>US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels</b>	27/03/2009	Air	1	ug day <sup>-1</sup>	Exposure to methylnaphthalenes is mainly by inhalation. The estimated average daily intake from ambient air may be about 1µg. Estimate is based on ambient air samples taken from 17 locations and assuming human daily intake of 20 m <sup>3</sup>	Shah and Heyerdahl 1988 in Research Triangle Institute. 1995. TOXICOLOGICAL PROFILE FOR NAPHTHALENE, 1-METHYLNAPHTHALENE, AND 2-METHYLNAPHTHALENE. Prepared for: U.S. DEPARTMENT OF HEALTH AND HUMAN SERVICES Public Health Service Agency for Toxic Substances and Disease Registry ( <a href="http://72.30.186.56/search/cache?ei=UTF-8&amp;p=NAPHTHALENE%2C+1-METHYLNAPHTHALENE%2C+AND+2-METHYLNAPHTHALENE&amp;rd=r1&amp;fr=yfp-t-501&amp;u=www.regulations.gov/fdmspublic/ContentViewer%3FobjectId%3D09000064800c0b6d%26disposition%3Dattachment%26contentType%3Dpdf&amp;w=naphthalene+1+methylnaphthalene+2+methylnaphthalene&amp;d=MPzhTExISdsK&amp;icp=1&amp;.intl=uk">http://72.30.186.56/search/cache?ei=UTF-8&amp;p=NAPHTHALENE%2C+1-METHYLNAPHTHALENE%2C+AND+2-METHYLNAPHTHALENE&amp;rd=r1&amp;fr=yfp-t-501&amp;u=www.regulations.gov/fdmspublic/ContentViewer%3FobjectId%3D09000064800c0b6d%26disposition%3Dattachment%26contentType%3Dpdf&amp;w=naphthalene+1+methylnaphthalene+2+methylnaphthalene&amp;d=MPzhTExISdsK&amp;icp=1&amp;.intl=uk</a> )	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>



<b>2-Methylphenol</b>	<b>CAS Number:</b>	<b>95-48-7</b>	<b>Assessor A:</b>	Mathew Rouge	<b>Assessor B:</b>	Gareth Wills	<b>Final Review:</b>	Panel/SF
	<b>Date:</b>	March 09			<b>Date:</b>	April 09		28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	TDloral applied to oral, dermal and inhalation routes. Insufficient data to assess non threshold effects, so HCV based on threshold effects.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	100	ug.kg-1.d-1	Most recent and longer term study data used (ATSDR value for total cresols)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
IPCS INCHEM	<a href="http://inchem.org/">http://inchem.org/</a>	1995	Mar-09	Acceptable Daily Intake for cresols	0.17	mg/kg/d	170	No info.	NOAEL	50	mg/kg/d	300	10 for interspecies variation; 10 to account for the lack of chronic toxicity studies and possible genotoxic and promoting activity of cresols and 3 to account for intraspecies variation based on the rapid and complete metabolism	Not provided
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	TDI	0.05	mg/kg/d	50	No info.	LOAEL	50	mg/kg/d	1000	10 for interspecies, 10 for intraspecies variability and 10 for the lack of a NOAEL	Rats gavaged daily with p-cresol, o-cresol
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	Minimal Risk Level (NOAEL) for cresols. Also provides IRIS RfD below for o-cresol	0.1	mg/kg/d	100	No info.	LOAEL	100	mg/kg/d	1000	10 for extrapolation from animals to humans, 10 for human variability and 10 for use of LOAEL	chronic oral study in female mice (NTP,2008)
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1990	Mar-09	RfD	0.05	mg/kg/d	50	Study - High, Database - Med, RfD - Med	NOAEL	50	mg/kg/d	1000	10 for interspecies, 10 for intraspecies variability and 10 for uncertainty in extrapolation of subchronic data to levels of chronic effects	Rats gavaged daily with p-cresol, o-cresol

TDI inhal	Recommended TDlinhal	Units	Justification
	N/A	ug.kg-1.d-1	Insufficient data with sufficient detail to derive HCV

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	Tolerable concentration in air (TCA)	170	ug/m3	50	TCA is provisional	Not provided	No study				
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No derivation of inhalation MRL because the inhalation data are inadequate to establish concentration-response relationships	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	Insufficient information exists to derive an RfC	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rr.html">http://www.tceq.state.tx.us/remediation/rr.html</a>	2008	May-09	RS ESL	0.01	mg/m3	2.857	Not Provided	Not Provided	Not Provided	Not Provided	Not Provided	Not Provided	Not Provided

**2-Methylphenol**

TDI oral
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Organisation	Description	Target organ/Critical Effect	Reference	Web link
IPCS INCHEM	Based on the results of subchronic studies, although no further information provided	Not provided	Not provided	<a href="http://incchem.org/documents/ehc/ehc/ehc168.htm">http://incchem.org/documents/ehc/ehc/ehc168.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	90 day subchronic toxicity study (US EPA, 1986), rats gavaged daily with p-cresol. 90 day neurotoxicity study (US EPA, 1987), rats gavaged daily with o-cresol	CNS, Weight loss, neurological events	US EPA. 1986/1987. o,m,p-cresol.90-Day oral subchronic/neurotoxicity toxicity study in rats. Office of Solid Waste, Washington, DC	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Groups of female mice were administered m/p-cresol (60% m-cresol, 40% p-cresol) in the diet at levels of 0,1000,3000 or10,000 ppm for 2 years (NTP 2008)	Lung/thyroid. LOAEL of 100 mg/kg/d for bronchiolar hyperplasia & thyroid follicular	NTP,2008. Toxicology and carcinogenesis studies of cresols (CAS No. 1319-77-3) in male F344/N rats and female B6C3F1 mice (feed studies). Research Triangle Park, NC: National Toxicology Program. TR-550. Draft technical report.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	90 day subchronic toxicity study (US EPA, 1986), rats gavaged daily with p-cresol. 90 day neurotoxicity study (US EPA, 1987), rats gavaged daily with o-cresol	CNS, Weight loss, neurological events	US EPA. 1986/1987. o,m,p-cresol.90-Day oral subchronic/neurotoxicity toxicity study in rats. Office of Solid Waste, Washington, DC	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

TDI inhal
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Organisation	Description	Response	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	TCA was calculated from multiplication of TDI (50 ug/kg/d) by 70kg (mean adult body weight) and divided by 20 m3 (mean adult breathing rate). TCA is provisional because it is derived via route-to-route extrapolation	Not provided	Not provided	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	The health effects data for 2-methylphenol were reviewed by the U.S. EPA RfD/RfC Work Group and determined to be inadequate for the derivation of an inhalation RfC. The verification status for this chemical is currently not verifiable	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>
Texas Commission on Environmental Quality	Not Provided	Not Provided	Not Provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>

<b>2-Methylphenol</b>	<b>CAS Number:</b>	<b>95-48-7</b>	<b>Assessor A:</b>	Mathew Rouge	<b>Assessor B:</b>	Gareth Wills	<b>Final Review:</b>	Panel/SF
			<b>Date:</b>	March 09	<b>Date:</b>	April 09	<b>Date:</b>	28/08/2009

<b>ID oral</b>	<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>
	N/A		No quantitative estimate of carcinogenic risk from oral exposure

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis	Study type	
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No quantitative estimate of carcinogenic risk from oral exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	No quantitative estimate of carcinogenic risk from oral exposure. Carcinogenic Classification C; possible human carcinogen	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	31/01/2002	Jul-09	A provisional oral slope factor cannot be derived because human and animal oral cancer data are lacking.	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

<b>ID inhal</b>	<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>
	N/A		No quantitative estimate of carcinogenic risk from inhalation exposure

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis	Study type	
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No quantitative estimate of carcinogenic risk from inhalation exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	No quantitative estimate of carcinogenic risk from inhalation exposure. Carcinogen Classification - C; possible human carcinogen	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

**2-Methylphenol**

ID oral
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Organisation	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	n/a	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>

ID inhal
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Organisation	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

<b>2-Methylphenol</b>	CAS 95-48-7	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
		Date	08/04/2009	Date	15/04/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, background exposure assumed negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 3500µg/L based on a 70kg adult consuming 2L/day.
	<b>0</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Environmental Health Criteria (EHC) Monographs	1995	air, drinking water, food	No data		Due to the lack of adequate monitoring data, it is not possible to estimate the daily intake of cresols from these sources	Cresols - (Environmental health criteria ; 168) ISBN 92 4 157168 1 (NLM Classification: QV 223) ISSN 0250-863X	<a href="http://inchem.org/documents/ehc/ehc/ehc168.htm">http://inchem.org/documents/ehc/ehc/ehc168.htm</a>
		drinking water	No data		No quantitative data available regarding cresol levels in drinking water in USA are available		

<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Cresols not widely occurring atmospheric pollutants. ATSDR data selected as most representative of background exposure = 31.7ng/m3 converted assuming an adult breathes 20m3/day.
	<b>0.634</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Environmental Health Criteria (EHC) Monographs	1995	Ambient Air	31.8	ug day-1	Environmental Health Criteria 168 - Reports the median air concentration of o-cresols was 1.59 µg/m3 (0.359 ppb) for 32 source-dominated sites in the USA. This converts to 31.8 ug day based on the CLEA calculations (20 m3 day air)	Cresols - (Environmental health criteria ; 168) ISBN 92 4 157168 1 (NLM Classification: QV 223) ISSN 0250-863X	<a href="http://inchem.org/documents/ehc/ehc/ehc168.htm">http://inchem.org/documents/ehc/ehc/ehc168.htm</a>
		air	100000	ug day-1	In air samples from rooms with a fireplace, cresol concentrations around 5 mg/m3 have been detected. This converts to 100,000 ug day based on the CLEA calculations (20 m3 day air)		
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	2000	Ambient Air	0.634	ug day-1	Monitoring data have not shown cresols to be widely occurring atmospheric pollutants. A national emissions study conducted from 1990 to 1998 reported an estimated ambient concentration average of 31.7 ng/m3	EPA. 2000. National air pollutant emission trends, 1900-1998. Research Triangle Park, NC: U.S. <a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp34.pdf</a>	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
Toxicological Data Network (TOXNET)	1993	Ambient Air	1.4	ug day-1	Mean concn of 0.07 ug/m3 (range, 0-0.13 ug/m3) in the US - converted to 1.4ug day, using CLEA intake value of 20 m3 a day	Kelly TJ et al; Ambient Concentration Summaries for Clean Air Act Title III Hazardous Air Pollutants. USEPA/600/R-94/090 Final Report Research Triangle Park (1993)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~rMogaz:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~rMogaz:1</a>

Substance:	<b>2-Methylphenol (o-Cresol)</b>	CAS Number:	95-48-7	Assessor A:	Mathew Rouge	Assessor B:	Gareth Wills	Final Review:	Panel/SF
Chemical Formula:	C7H8O	Phase at Ambient Temperature:	Solid	Date:	25/03/2009	Date:	30/04/2009	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oecd.org/scripts/hpv/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000							
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)		
<b>Required Parameters</b>																																			
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	108.138	n/a	central value from consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)		
						Average	108.15	108.15	n/a	108.138	108.138	n/a	108.138	108.138	n/a	108.14	108.14	n/a	108.14	108.14	n/a	108.14	108.14	n/a	108.1378	108.1378	n/a	108.2	108.2	n/a	108.2	108.2	n/a		
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	1.45E-01	25	Values not in consistent range. Most recent value selected		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	kPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)		
						Geomean	1.60E-06	1.62E-01	25	No info.	#VALUE!	25	1.24E-01	1.24E-01	25	1.56E-01	25	1.45E-01	25	#VALUE!	25	#VALUE!	25	1.20E-06	0.12159	25	1.20E+03	8.36E-02	25	1.42E-01	25	#VALUE!	25		
				</																															

<b>Contaminant Name: 3-Methylphenol</b>	<b>CAS Number:</b> 108-39-4	<b>Assessor A:</b> Mathew Rouge	<b>Assessor B:</b> Gareth Wills	<b>Final Review:</b>	<b>Panel/SF</b>
		<b>Date:</b> Mar-09	<b>Date:</b> Apr-09	<b>Date:</b> 28/08/2009	

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	TDloral applied to oral, dermal and inhalation routes. Insufficient data to assess non threshold effects, so HCV based on threshold effects.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	100	µg.kg-1.d-1	Most recent and longer term study data used (ATSDR value for total cresols)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
IPCS INCHEM	<a href="http://incem.org/">http://incem.org/</a>	1995	Mar-09	Acceptable Daily Intake for cresols	0.17	mg/kg/d	170	No info.	NOAEL	50	mg/kg/d	300	10 for interspecies variation; 10 to account for the lack of chronic toxicity studies and possible genotoxic and promoting activity of cresols and 3 to account for intraspecies variation based on the rapid and complete metabolism
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	TDI	0.05	mg/kg/d	50	No info.	LOAEL	50	mg/kg/d	1000	10 for interspecies, 10 for intraspecies variability and 10 for the lack of a NOAEL
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	Minimal Risk Level (NOAEL) for cresols. Also provides IRIS RfD below for o-cresol	0.1	mg/kg/d	100	No info.	LOAEL	100	mg/kg/d	1000	10 for extrapolation from animals to humans, 10 for human variability and 10 for use of LOAEL
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1990	Mar-09	RfD	0.05	mg/kg/d	50	Study - High, Database - Med, RfD - Med	NOAEL	50	mg/kg/d	1000	10 for interspecies, 10 for intraspecies variability and 10 for uncertainty in extrapolation of subchronic data to levels of chronic effects

TDI inhal	Recommended TDlinhal	Units	Justification
	N/A	µg.kg-1.d-1	Insufficient data with sufficient detail to derive HCV

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	Tolerable concentration in air (TCA)	170	ug/m3	50	TCA is provisional	Not provided				
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No derivation of inhalation MRL because the inhalation data are inadequate to establish concentration-response relationships	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	Insufficient information exists to derive an RfC	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Contaminant Name: 3-Methylphenol

TDI oral						
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link	
IPCS INCHEM	Not provided	Based on the results of subchronic studies, although no further information provided	Not provided	Not provided	<a href="http://incem.org/documents/ehc/ehc/ehc168.htm">http://incem.org/documents/ehc/ehc/ehc168.htm</a>	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Rats gavaged daily with p-cresol, o-cresol	90 day subchronic toxicity study (US EPA, 1986), rats gavaged daily with p-cresol. 90 day neurotoxicity study (US EPA, 1987), rats gavaged daily with o-cresol	CNS, Weight loss, neurological events	US EPA. 1986/1987. o,m,p-cresol.90-Day oral subchronic/neurotoxicity toxicity study in rats. Office of Solid Waste, Washington, DC	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	chronic oral study in female mice (NTP,2008)	Groups of female mice were administered m/p-cresol (60% m-cresol, 40% p-cresol) in the diet at levels of 0,1000,3000 or10,000 ppm for 2 years (NTP 2008)	Lung/thyroid. LOAEL of 100 mg/kg/d for bronchiolar hyperplasia & thyroid follicular	NTP,2008. Toxicology and carcinogenesis studies of cresols (CAS No. 1319-77-3) in male F344/N rats and female B6C3F1 mice (feed studies). Research Triangle Park, NC: National Toxicology Program. TR-550. Draft technical report.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>	
USEPA Integrated Risk Information System (IRIS)	Rats gavaged daily with p-cresol, o-cresol	90 day subchronic toxicity study (US EPA, 1986), rats gavaged daily with p-cresol. 90 day neurotoxicity study (US EPA, 1987), rats gavaged daily with o-cresol	CNS, Weight loss, neurological events	US EPA. 1986/1987. o,m,p-cresol.90-Day oral subchronic/neurotoxicity toxicity study in rats. Office of Solid Waste, Washington, DC	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	
TDI inhal						
Organisation	Study type	Description	Response	Reference	Web link	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	No study	TCA was calculated from multiplication of TDI (50 ug/kg/d) by 70kg (mean adult body weight) and divided by 20 m3 (mean adult breathing rate). TCA is provisional because it is derived via route-to-route extrapolation	Not provided	Not provided	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>	
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	The health effects data for 3-methylphenol were reviewed by the U.S. EPA RfD/RfC Work Group and determined to be inadequate for the derivation of an inhalation RfC. The verification status for this chemical is currently not verifiable	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	

<b>Contaminant Name: 3-Methylphenol</b>		<b>CAS Number:</b>	<b>108-39-4</b>	<b>Assessor A:</b>	Mathew Rouge	<b>Assessor B:</b>	Gareth Wills	<b>Final Review:</b>		<b>Panel/SF</b>	
<b>Other (Texas Commission on Environmental Quality)</b>		<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>	2008	Mar-09	RS-ESL	0.01 mg/m3	2.857	Not provided	Not provided	Not provided	Not provided

<b>ID oral</b>	<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>
	N/A		No quantitative estimate of carcinogenic risk from oral exposure

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis		
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No quantitative estimate of carcinogenic risk from oral exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	No quantitative estimate of carcinogenic risk from oral exposure. Carcinogenicity Classification C; possible human carcinogen	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2002	Jul-09	A provisional oral slope factor cannot be derived because human and animal oral cancer data are lacking.	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

<b>ID inhal</b>	<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>
	N/A		No quantitative estimate of carcinogenic risk from inhalation exposure

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis		
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No quantitative estimate of carcinogenic risk from inhalation exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	No quantitative estimate of carcinogenic risk from inhalation exposure. Carcinogenicity Classification C; possible human carcinogen	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

**Contaminant Name: 3-Methylphenol**

Other (Texas Commission on Environmental Quality)	Not provided	Not provided	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>
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**ID oral**

Organisation	Study type	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	n/a	n/a	n/a	n/a	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>

**ID inhal**

Organisation	Study type	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

<b>3-Methylphenol</b>	CAS 108-39-4	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
		Date	08/04/2009	Date	15/04/2009	Date	28/08/2009

MDI			Recommended MDI <sub>oral</sub>	Units	Justification: No data, background exposure assumed negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 3500µg/L based on a 70kg adult consuming 2L/day.		
			0	ug day-1			
Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Environmental Health Criteria (EHC) Monographs	1995	air, drinking water, food	No data		Due to the lack of adequate monitoring data, it is not possible to estimate the daily intake of cresols from these sources	Cresols - (Environmental health criteria ; 168) ISBN 92 4 157168 1 (NLM Classification: QV 223) ISSN 0250-863X	<a href="http://inchem.org/documents/ehc/ehc/ehc168.htm">http://inchem.org/documents/ehc/ehc/ehc168.htm</a>
		drinking water	No data		No quantitative data available regarding cresol levels in drinking water in USA are available		

MDI			Recommended MDI <sub>inh</sub>	Units	Justification: Cresols not widely occurring atmospheric pollutants. ATSDR data selected as most recent representative of background exposure = 31.7ng/m3 converted assuming an adult breathes 20m3/day.		
			0.634	ug day-1			
Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Environmental Health Criteria (EHC) Monographs	1995	air	100000	ug day-1	In air samples from rooms with a fireplace, cresol concentrations around 5 mg/m3 have been detected. This converts to 100,000 ug day based on the CLEA calculations (20 m3 day air)	Risner CH (1993) The quantification of hydroquinone, catechol, phenol,3-methylcatechol, scopoletin, <i>m+p</i> - cresol and <i>o</i> - cresol in indoor air sample by high performance liquid chromatography. J LiqChromatogr, 16:4117-4140.	<a href="http://inchem.org/documents/ehc/ehc/ehc168.htm">http://inchem.org/documents/ehc/ehc/ehc168.htm</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	2000	Ambient Air	0.634	ug day-1	Monitoring data have not shown cresols to be widely occurring atmospheric pollutants. A national emissions study conducted from 1990 to 1998 reported an estimated ambient concentration average of 31.7 ng/m3	EPA. 2000. National air pollutant emission trends, 1900-1998. Research Triangle Park, NC: U.S. <a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp34.pdf</a>	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
Toxicological Data Network (TOXNET)	1993	Ambient Air	28	ug day-1	Combined m,p-cresol isomers mean concn of 1.4 ug/m3 (range, 0-4.1 ug/m3) in the US - converted to 28ug day, using CLEA intake value of 20 m3 a day	Kelly TJ et al; Ambient Concentration Summaries for Clean Air Act Title III Hazardous Air Pollutants. USEPA/600/R-94/090 Final Report Research Triangle Park (1993)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/?/~VaK2Cn:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/?/~VaK2Cn:1</a>



<b>4-Methylphenol</b>	<b>CAS Number:</b> 106-44-5	<b>Assessor A:</b> Mathew Rouge	<b>Assessor B:</b> Gareth Wills	<b>Final Review:</b>	<b>Panel/SF</b>
		<b>Date:</b> Mar-09	<b>Date:</b> Apr-09	<b>Date:</b> 28/08/2009	

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	TDloral applied to oral, dermal and inhalation routes. Insufficient data to assess non threshold effects, so HCV based on threshold effects.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	100	ug.kg-1.d-1	Most recent and longer term study data used (ATSDR value for total cresols)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg.1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
IPCS INCHEM	<a href="http://inchem.org/">http://inchem.org/</a>	1995	Mar-09	Acceptable Daily Intake for cresols	0.17	mg/kg/d	170	No info.	NOAEL	50	mg/kg/d	300	10 for interspecies variation; 10 to account for the lack of chronic toxicity studies and possible genotoxic and promoting activity of cresols and 3 to account for intraspecies variation based on the rapid and complete metabolism	Not provided
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	TDI	0.05	mg/kg/d	50	No info.	LOAEL	50	mg/kg/d	1000	10 for interspecies, 10 for intraspecies variability and 10 for the lack of a NOAEL	Rats gavaged daily with p-cresol, o-cresol
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	Minimal Risk Level (NOAEL) for cresols	0.1	mg/kg/d	100	No info.	LOAEL	100	mg/kg/d	1000	10 for extrapolation from animals to humans, 10 for human variability and 10 for use of LOAEL	chronic oral study in female mice (NTP,2008)
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		Mar-09	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rr.html">http://www.tceq.state.tx.us/remediation/rr.html</a>	2008	Mar-09	RfD	5	ug/kg bw/d	5	No info.	NOAEL	Not provided	Not provided	Not provided	Not provided	Not provided

TDI inhal	Recommended TDlinhal	Units	Justification
	N/A	ug.kg-1.d-1	Insufficient data with sufficient detail to derive HCV

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg.1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	Tolerable concentration in air (TCA)	170	ug/m3	48.57	TCA is provisional	Not provided	50	ug/kg/d	Not provided	Not provided	No study
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No derivation of inhalation MRL because the inhalation data are inadequate to establish concentration-response relationships	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

**4-Methylphenol****TDI oral**

Organisation	Description	Target organ/Critical Effect	Reference	Web link
IPCS INCHEM	Based on the results of subchronic studies, although no further information provided	Not provided	Not provided	<a href="http://incchem.org/documents/ehc/ehc/ehc168.htm">http://incchem.org/documents/ehc/ehc/ehc168.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	90 day subchronic toxicity study (US EPA, 1986), rats gavaged daily with p-cresol. 90 day neurotoxicity study (US EPA, 1987), rats gavaged daily with o-cresol	CNS, Weight loss, neurological events	US EPA. 1986/1987. o,m,p-cresol.90-Day oral subchronic/neurotoxicity toxicity study in rats. Office of Solid Waste, Washington, DC	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Groups of female mice were administered m/p-cresol (60% m-cresol, 40% p-cresol) in the diet at levels of 0,1000,3000 or10,000 ppm for 2 years (NTP 2008)	Lung/thyroid. LOAEL of 100 mg/kg/d for bronchiolar hyperplasia & thyroid follicular	NTP,2008. Toxicology and carcinogenesis studies of cresols (CAS No. 1319-77-3) in male F344/N rats and female B6C3F1 mice (feed studies). Research Triangle Park, NC: National Toxicology Program. TR-550. Draft technical report.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>
Texas Commission on Environmental Quality	The value was taken from USEPA Health Effects Assessment Summary Tables (HEAST), July 1997	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>

**TDI inhal**

Organisation	Description	Response	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	TCA was calculated from multiplication of TDI (50 ug/kg/d) by 70kg (mean adult body weight) and divided by 20 m3 (mean adult breathing rate). TCA is provisional because it is derived via route-to-route extrapolation	Not provided	Not provided	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>

<b>4-Methylphenol</b>		<b>CAS Number:</b>	<b>106-44-5</b>	<b>Assessor A:</b>	<b>Mathew Rouge</b>	<b>Assessor B:</b>	<b>Gareth Wills</b>	<b>Final Review:</b>						<b>Panel/SF</b>
				<b>Date:</b>	<b>Mar-09</b>	<b>Date:</b>	<b>Apr-09</b>	<b>Date:</b>						<b>28/08/2009</b>
<b>USEPA Integrated Risk Information System (IRIS)</b>	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	Insufficient information exists to derive an RFC	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
<b>Texas Commission on Environmental Quality</b>	<a href="http://www.tceq.state.tx.us/remediation/rr.html">http://www.tceq.state.tx.us/remediation/rr.html</a>	2008	Mar-09	RS-ESL	0.01	mg/m3	2.857	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided

<b>ID oral</b>	<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>
	N/A		No quantitative estimate of carcinogenic risk from oral exposure

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis	Study type
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No quantitative estimate of carcinogenic risk from oral exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	No quantitative estimate of carcinogenic risk from oral exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

<b>ID inhal</b>	<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>
	N/A		No quantitative estimate of carcinogenic risk from inhalation exposure

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis	Study type
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	2008	Mar-09	No quantitative estimate of carcinogenic risk from inhalation exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1991	Mar-09	No quantitative estimate of carcinogenic risk from inhalation exposure	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

**4-Methylphenol**

USEPA Integrated Risk Information System (IRIS)	n/a	n/a	The health effects data for 4-methylphenol were reviewed by the U.S. EPA RfD/RfC Work Group and determined to be inadequate for the derivation of an inhalation RfC. The verification status for this chemical is currently not verifiable.	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>
Texas Commission on Environmental Quality	Not provided	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>

## ID oral

Organisation	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

## ID inhal

Organisation	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

<b>4-Methylphenol</b>	CAS 106-44-5	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
		Date	08/04/2009	Date	15/04/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, background exposure assumed negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 3500µg/L based on a 70kg adult consuming 2L/day.
	<b>0</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Environmental Health Criteria (EHC) Monographs	1995	air, drinking water, food	No data		Due to the lack of adequate monitoring data, it is not possible to estimate the daily intake of cresols from these sources	Cresols - (Environmental health criteria ; 168) ISBN 92 4 157168 1 (NLM Classification: QV 223) ISSN 0250-863X	<a href="http://inchem.org/documents/ehc/ehc/ehc168.htm">http://inchem.org/documents/ehc/ehc/ehc168.htm</a>
		drinking water	No data		No quantitative data available regarding cresol levels in drinking water in USA are available		

<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Cresols not widely occurring atmospheric pollutants. ATSDR data selected as most recent representative of background exposure = 31.7ng/m <sup>3</sup> converted assuming an adult breathes 20m <sup>3</sup> /day.
	<b>0.634</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Environmental Health Criteria (EHC) Monographs	1995	air	100000	ug day-1	in air samples from rooms with a fireplace, cresol concentrations around 5 mg/m <sup>3</sup> have been detected. This converts to 100,000 ug day based on the CLEA calculations (20 m <sup>3</sup> day air)	Risner CH (1993) The quantification of hydroquinone, catechol, phenol, 3-methylcatechol, scopoletin, <i>m+p</i> -cresol and <i>o</i> -cresol in indoor air sample by high performance liquid chromatography. <i>J LiqChromatogr</i> , 16:4117-4140.	<a href="http://inchem.org/documents/ehc/ehc/ehc168.htm">http://inchem.org/documents/ehc/ehc/ehc168.htm</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	2000	Ambient Air	0.634	ug day-1	Monitoring data have not shown cresols to be widely occurring atmospheric pollutants. A national emissions study conducted from 1990 to 1998 reported an estimated ambient concentration average of 31.7 ng/m <sup>3</sup>	EPA. 2000. National air pollutant emission trends, 1900-1998. Research Triangle Park, NC: U.S. <a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp34.pdf</a>	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp34.html">http://www.atsdr.cdc.gov/toxprofiles/tp34.html</a>
Toxicological Data Network (TOXNET)	1993	Ambient Air	28	ug day-1	Combined <i>m,p</i> -cresol isomers mean concn of 1.4 ug/m <sup>3</sup> (range, 0-4.1 ug/m <sup>3</sup> ) in the US - converted to 28ug day, using CLEA intake value of 20 m <sup>3</sup> a day	Kelly TJ et al; Ambient Concentration Summaries for Clean Air Act Title III Hazardous Air Pollutants. USEPA/600/R-94/090 Final Report Research Triangle Park (1993)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/temp/~VaK2Cn:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/temp/~VaK2Cn:1</a>

Substance:		4-Methylphenol (p-Cresol)		CAS Number:		106-44-5		Assessor A:		Mathew Rouge		Assessor B:		Gareth Wills		Final Review:		Panel/SF															
Chemical Formula:		C7H8O		Phase at Ambient Temperature:		Solid		Date:		25/03/2009		Date:		30/04/2009		Date:		28/08/2009															
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H					
							HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCK, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000					
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)			
<b>Required Parameters</b>																																	
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	108.138	n/a	central value selected from consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)			
Average							108.13	108.13	n/a	108.138	108.138	n/a	108.138	108.138	n/a	108.14	108.14	n/a	108.14	108.14	n/a	108.14	108.14	n/a	108.1378	108.1378	n/a	108.2	108.2	n/a			
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	1.37E-01	25	values not in consistent range. Newest value selected		atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	KPa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	Pa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)			
Geomean							9.60E-07	9.73E-02	25	No info.	#VALUE!	25	#VALUE!	25	8.02E-02	0.0802	25	1.21E-01	25	7.69E-07	0.077918925	25	No info.	#VALUE!	25	2.50E+03	4.01E-02	25	8.86E-02	25			
Average							0.0699	0.0699	25	0.0699	0.0699	25	0.0699	0.0699	25	n/a	n/a	25	n/a	n/a	25	0.00000343	0.34754475	25	0.00000343	0.34754475	25	1100	9.12E-02	25	1100	9.12E-02	25
Average							0.0973	0.0973	25	0.0973	0.0973	25	0.0973	0.0973	25	n/a	n/a	25	n/a	n/a	25	0.0973	0.0973	25	0.0973	0.0973	25	520	1.93E-01	25	520	1.93E-01	25
Average							0.0397	0.0397	25	0.0397	0.0397	25	0.0397	0.0397	25	n/a	n/a	25	n/a	n/a	25	0.0397	0.0397	25	0.0397	0.0397	25	1000	1.00E-01	25	1000	1.00E-01	25
Average							0.0653	0.0653	25	0.0653	0.0653	25	0.0653	0.0653	25	n/a	n/a	25	n/a	n/a	25	0.0653	0.0653	25	0.0653	0.0653	25	1300	7.72E-02	25	1300	7.72E-02	25
Average							0.0783	0.0783	25	0.0783	0.0783	25	0.0783	0.0783	25	n/a	n/a	25	n/a	n/a	25	0.0783	0.0783	25	0.0783	0.0783	25	n/a	n/a	25	n/a	n/a	25
Average							0.081	0.081	25	0.081	0.081	25	0.081	0.081	25	n/a	n/a	25	n/a	n/a	25	0.081	0.081	25	0.081	0.081	25	n/a	n/a	25	n/a	n/a	25
Average							0.0989	0.0989	25	0.0989	0.0989	25	0.0989	0.0989	25	n/a	n/a	25	n/a	n/a	25	0.0989	0.0989	25	0.0989	0.0989	25	n/a	n/a	25	n/a	n/a	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	2.34E+04	25	values not in consistent range. Newest value closest to 10 degrees selected		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)			
Geomean							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25	2.20E+04	2.20E+04	25	No info.	#VALUE!	25	No info.	#VALUE!	25
Average							2.26E+04	2.26E+04	40	2.31E+01	23100	40	2.31E+01	23100	40	2.42E+04	2.42E+04	25	2.15E+04	21500	25	No info.	#VALUE!	25									

Biphenyl	CAS Number:	92-52-4	Assessor A:	Y Macklin, AMEC	Assessor B:	K Privett, Hydrock	Final review:	Panel/SF
			Date	25/03/2009	Date	08/05/2009	Date	26/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	Classification D (IRIS) not classifiable as to human carcinogenicity. Insufficient data with sufficient detail to derive inhalation HCV. Use route-to-route extrapolation from oral.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	38	ug.kg-1.d-1	CICAD value taken even though provisional status, and is more recent than IRIS value

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	unknown	26/03/2009	Provisional TDI	0.038	mg/kg bw/day	38	Provisional	LOEL	38	mg/kg bw/day	1000
JECFA 2	<a href="http://inchem.org/pages/jecfa.html">http://inchem.org/pages/jecfa.html</a>	unknown	27/03/2009	TDI	0.05	mg/kg bw/day	50		Acceptable daily intake for a man (unconditional acceptance).	0.05	mg/kg bw/day	not given
JMPR 2	<a href="http://inchem.org/pages/jmpr.html">http://inchem.org/pages/jmpr.html</a>	unknown	27/03/2009	TDI	0.125	mg/kg bw/day	125		Acceptable daily intake for a 60kg person.			
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	02/07/2008	27/03/2009	MOE	25000				Based on a LOEL of 38 mg/kg bw/day and a daily intake of biphenyl of 1.5 mg/kg bw/day	38	mg/kg bw/day	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	10/01/2008	27/03/2009	RfD	5.00E-02	mg/kg bw/day	50		NOAEL	50	mg/kg bw/day	100

Biphenyl

TDI oral						
Organisation	UF description	Study type	Description	Target organ/Critical Effect	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)	x10 for interspecies variation, x10 for intraspecies variation, x10 for extrapolation from a LOEL to a NOEL.	Animal	Based on the development effects on the blood of rats administered diets containing biphenyl for 2 years.		WHO (1999) Concise International Chemical Assessment Document 6. Biphenyl.	<a href="http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf">http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf</a>
JECFA 2			Long term study in rats use of dietary levels of 0.01%, 0.1% and 1% diphenyl for a 2-year period.		Joint FAO/WHO Expert Committee on Food Additives (1964) Specifications for identify and purity and toxicological evaluation of some antimicrobials and antioxidants	<a href="http://www.inchem.org/documents/jecfa/jecmono/v38aje15.htm">http://www.inchem.org/documents/jecfa/jecmono/v38aje15.htm</a>
JMPR 2	not given		not given	not given	Joint Meeting of the FAO Working Party and the WHO Expert Committee on Pesticide Residues (1967) EVALUATION OF SOME PESTICIDE RESIDUES IN FOOD	<a href="http://www.inchem.org/documents/jmpr/jmpmono/v66apr07.htm">http://www.inchem.org/documents/jmpr/jmpmono/v66apr07.htm</a>
Health Canada Toxicological Values	not given	Animal-chronic	Lowest oral (diet) non-neoplastic LOEL (rat) = 38 mg/kg-bw per day: increased serum enzyme and blood urea nitrogen levels (2-year study).		(Japan Bioassay Research Center,1996; Umeda et al., 2002) in Health Canada (2005) State of the Science Report for a Screening Health Assessment- 1,1-Biphenyl	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/biphenyl-biphenyle/biphenyl-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/biphenyl-biphenyle/biphenyl-eng.pdf</a>
USEPA Integrated Risk Information System (IRIS)	UF — Factors of 10 each for interspecies conversion and for protection of sensitive human subpopulations were applied to the NOAEL of 50 mg/kg/day. An additional factor of 10 was applied to account for intraspecies variability demonstrated by uncertainty in the threshold suggested by the data in the critical study.	Rat Chronic Oral Study	15 weanling albino rats of each sex were placed in each of 8 experimental groups: 0.0, 0.001, 0.005, 0.01, 0.05, 0.10, 0.50, and 1.0% biphenyl in the diet. Dietary levels of 0.5% biphenyl and greater were associated with kidney damage, reduced haemoglobin levels, decreased food intake, and decreased longevity. One animal in each of the lower dose groups and control group had detectable blood in the renal pelvis. A supporting unpublished work (SRI, 1960) was cited in which a NOAEL of 0.1% biphenyl in the diet was found in both a subchronic rat feeding study and a three- generation rat reproduction study.	Kidney damage	Ambrose, A.M., A.N. Booth, F. DeEds and A.J. Cox, Jr. 1960. A toxicological study of biphenyl, a citrus fungistat. Food Res. 25: 328-336	<a href="http://www.epa.gov/NCEA/iris/subst/0013.htm">http://www.epa.gov/NCEA/iris/subst/0013.htm</a>

Biphenyl		CAS Number: 92-52-4		Assessor A: Y Macklin, AMEC		Assessor B: K Privett, Hydrock		Final review: Panel/SF				
				Date	25/03/2009	Date	08/05/2009	Date	26/08/2009			
<b>TDI inhal</b>				<b>Recommended TDIinhal</b>	<b>Units</b>	<b>Justification</b>						
						Insufficient data with sufficient detail to derive HCV						
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	unknown	26/03/2009	OEL		1.3 mg/m3						
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	02/07/2008	27/03/2009						LOEC		5 mg/m3	
USEPA Acute Guideline Levels (AEGLS)	<a href="http://epa.gov/oppt/aegl/pubs/chemlist.htm">http://epa.gov/oppt/aegl/pubs/chemlist.htm</a>	13/02/2009	27/03/2009	OEL (AEG-2)	28 (8 Hour)	mg/m3			Derived from chronic mouse study			90?- not implicitly stated
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	10/01/2008	27/03/2009	The health effects data for biphenyl were reviewed by the U.S. EPA RfD/RfC Work Group and determined to be inadequate for derivation of an inhalation RfC								
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	unknown	27/03/2009	OEL 8-hrTWA		1 mg/m3			Not given. OSHA, ACGIH, NIOSH			
<b>ID oral</b>				<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>						
				n/a		Classification D (IRIS) not classifiable as to human carcinogenicity. No human data and inadequate studies in mice and rats. Results of genotoxicity tests are generally negative.						
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis
<b>ID inhal</b>				<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>						
				n/a		Classification D (IRIS) not classifiable as to human carcinogenicity. No human data and inadequate studies in mice and rats. Results of genotoxicity tests are generally negative.						
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis

Biphenyl

TDI inhal

Organisation	UF description	Study type	Description	Response	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)						<a href="http://inchem.org/documents/cicads/cicads/cicad06.htm#SubSectionNumber:8.3.2">http://inchem.org/documents/cicads/cicads/cicad06.htm#SubSectionNumber:8.3.2</a>
Health Canada Toxicological Values		Subchronic	Lowest-Observed-Effect Concentration (LOEC) for non-neoplastic effects (mortality and respiratory irritation) (5 mg/m <sup>3</sup> ) with the upper-bounding estimate of indoor air concentration (1 µg/m <sup>3</sup> ).			<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/biphenyl-biphenyle/evaluation-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/biphenyl-biphenyle/evaluation-eng.php</a>
USEPA Acute Guideline Levels (AEGs)	A total uncertainty factor of 10 was applied for the AEGL-2 values with 3 for interspecies variability because the mouse was the most sensitive species and had clinical signs similar to other species; and 3 for intraspecies variability.	Chronic-animal	chronic inhalation study in mice exposed to 316 mg/m <sup>3</sup> (50 ppm) biphenyl 7 hours/day, 5 days/week for 13 weeks. The report states some adverse clinical signs were observed but they are not stated. Upon histopathological examination, tracheal hyperplasia was recorded.		Cannon Laboratories, Inc. 1977. Final report: 90-day inhalation toxicity study of biphenyl (99+% purity) in CD-1 mice. Sponsored by Sun Company Lab. EPA Doc. No. 878213532; Fiche No. OTS0206401	<a href="http://epa.gov/oppt/aegl/pubs/rest147.htm">http://epa.gov/oppt/aegl/pubs/rest147.htm</a> and <a href="http://epa.gov/oppt/aegl/pubs/biphenyl_interim_11_2007.v1.pdf">http://epa.gov/oppt/aegl/pubs/biphenyl_interim_11_2007.v1.pdf</a>
USEPA Integrated Risk Information System (IRIS)						
Toxicology Data Network (Toxnet)			Based on NIOSH and OSHA occupational standards			

ID oral

Organisation	UF description	Study type	Description	Response	Reference	Web link
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ID inhal

Organisation	UF description	Study type	Description	Response	Reference	Web link
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Biphenyl	CAS 91-52-4	Assessor A:	Y Macklin, AMEC	Assessor B:	K Privett, Hydrock	Final review:	Panel/SF
		Date	25/03/2009	Date	08/05/2009	Date	26/08/2009

MDI	Recommended MDI <sub>oral</sub>	Units	Justification: Sum of dietary and water intake from CICAD document. Most relevant data in the absence of any UK data.
	4.49	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	06/04/2009	Drinking water	0.01	µg day <sup>-1</sup>	In measurements conducted in the 1970s, levels of biphenyl in tap-water were usually below 5 ng/litre. Multiply by 2l per day for adult consumption. Convert from ng/l to µg/l divide by 1,000.	<a href="http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf">http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf</a>	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	06/04/2009	Food	4.48	µg day <sup>-1</sup>	An average intake of 64 ng biphenyl/kg body weight per day from food was calculated based upon the consumption of foodstuffs in Finland. Original units (64 ng/kg bw/day) multiplied by 70kg to convert from ng/kg bw/day to ng/day. Convert from ng/day to µg/day divide by 1000.	<a href="http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf">http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf</a>	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Joint Expert Committee on Food Additives (JECFA)	28/01/2006	Food additive			No safety concern at current levels of intake when used as a flavouring agent.	TRS 928-JECFA 63/73 FAS 54-JECFA 63/291	<a href="http://iecfa.ilsa.org/evaluation.cfm?chemical=BIPHENYL&amp;keyword=BIPHENYL">http://iecfa.ilsa.org/evaluation.cfm?chemical=BIPHENYL&amp;keyword=BIPHENYL</a>
Joint FAO WHO Meeting on Pesticide Residues (JMPR)	06/04/2009	Food	100	ppm	Legal limit in citrus fruit for UK.	<a href="http://www.inchem.org/documents/jmpr/jmpmono/v66apr07.htm">http://www.inchem.org/documents/jmpr/jmpmono/v66apr07.htm</a>	<a href="http://www.who.int/ipcs/food/jmpr/en/">www.who.int/ipcs/food/jmpr/en/</a>
Health Canada Toxicological Reference Values	06/04/2009	Food, drinking water	1.5	µg/kg bw/day	The upper-bounding estimate of intake for the most highly exposed age group (i.e., 0.5–4 years) is 1.5 µg/kg bw per day for the general population.	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/biphenyl-biphenyle/biphenyl-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/biphenyl-biphenyle/biphenyl-eng.pdf</a>	<a href="http://www.hc-sc.gc.ca/index-eng.php">http://www.hc-sc.gc.ca/index-eng.php</a>
Toxicological Data Network (TOXNET)	23/08/2005	Drinking water			DWS MN 300ug/l FL 0.5ug/l	HSDB entry	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~9mdbn6:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~9mdbn6:1</a>
MDI	Recommended MDI <sub>inh</sub>	Units	Justification: in the absence of any UK data, CICAD data for Finland used.				
	0.524	ug day <sup>-1</sup>					

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	06/04/2009	Ambient air	0.524	µg day <sup>-1</sup>	In 1985, concentrations of biphenyl in the air of an industrialized city in Finland ranged from 1.7 to 26.2 ng/m <sup>3</sup> . Upper bound estimate used. Multiply by 20m <sup>3</sup> to allow for adult inhalation. Convert from ng/day to µg/day divide by 1,000.	<a href="http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf">http://www.who.int/ipcs/publications/cicad/en/cicad06.pdf</a>	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Health Canada Toxicological Reference Values	06/04/2009	Ambient air	3.50E-05	µg day <sup>-1</sup>	Table 1: Upper-bounding estimates of daily intake of biphenyl by the general population of Canada. Values for 0-6 months and 6months- 4 years added.	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/biphenyl-biphenyle/biphenyl-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/biphenyl-biphenyle/biphenyl-eng.pdf</a>	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>
Toxicological Data Network (TOXNET)	06/04/2009	Ambient air	2	µg day <sup>-1</sup>	In ambient air, typical concentrations of biphenyl range from 1 to 100 ng/m <sup>3</sup> . Upper end of range used. Convert to µg day multiply by 20m <sup>3</sup> and divide by 1000. No information provided on date or source of data.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~RQGBri:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~RQGBri:1</a>	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>





Bis ethylhexyl phthalate, di(2 ethylhexyl)phthalate or DEHP	CAS Number:	117-81-7	Assessor A: Barry Mitcheson, Enviros	Assessor B: Charlotte Clark, Hyder	Final review: Panel/SF	
	Date	05/05/2009	Date	06/05/2009	Date	26/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen - TDloral applied to oral, dermal and inhalation routes.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral					Recommended TDI oral	Units	Justification						
					50	ug.kg-1.d-1	Value selected by COT, ECB, EFSA & SCF. Lower values used by WHO and RIVM based upon discredited studies. Most recent value (2005) and is compatible with values referenced in several European sources. Other numbers are from American references						
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	5 August 2005 (One site date not given)	31/03/2009	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>	11-Sep-08	31/03/2009	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	29/4/8 (uploaded infant milk formula file from July 2006)	06/04/2009	TDI	0.05	mg/kgbw/day	50	Not given. Committee noted new evidence on reproductive effects published after these TDIs set.	Refers to SCF temporary "group restriction" of 0.05. COT notes TDIs derived from no effect dose in animals.			100	SCF not details given
Expert Panel on Air Quality Standards (EPAQS)	<a href="http://www.defra.gov.uk/environment/airquality/panels/ags/index.htm">http://www.defra.gov.uk/environment/airquality/panels/ags/index.htm</a>	N/A	07/04/2009	No data found	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search : 2005 Review of report by MS Technical Experts finalised: September 2005 Final report: 2008	07/04/2009	NOAEL for kidneys (14.5mg/kgbw/day), testicular (4.8mg/kgbw/day, reproduction (10mg/kgbw/day) development 4.8mg/kgbw/day) and added a MOS of 30 to 250 for adults to babies and 100 for children	0.145	mg/kgbw/day	145	Not given	Moore (1996) with adjustment for 50% absorption	14.5	NOAEL mg/kgbw/day	100	UF of 10 for species differences. UFs of 3 and 10 for intraspecies differences (worker and general population, respectively). Giving Margin of Safety of 30 (commercial) to 100 for children. 100 figure used. For infants of 3- 12 months a factor of 20, and for <3 months a factor of 250, was considered but noted that " all member states do not agree that newborns/infants need a higher margin of safety ".)
					0.048	mg/kgbw/day	48	Not given	Wolfe et al. (2003) Oral exposure	4.8	NOAEL mg/kgbw/day		
					0.1	mg/kgbw/day	100	Not given	Lamb et al. (1987) with adjustment for 50% absorption	10	NOAEL mg/kgbw/day		
					0.048	mg/kgbw/day	48	Not given	Wolfe et al. (2003) Oral exposure	4.8	NOAEL mg/kgbw/day		
European Food Safety Authority (EFSA)	<a href="http://www.efsa.europa.eu/en.html">http://www.efsa.europa.eu/en.html</a>			TDI	0.05	mg/kgbw/day	50		Based on effects potentially relevant to humans, authoritative body.	5	NOAEL mg/kg/bw/d	100	Not given

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di(2 ethylhexyl)phthalate or DEHP

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Food Standards Agency (FSA)	Data review	Reference to Endocrine disruptors. States that EFSA reviews all the scientific data to set a TDI. <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> - notes provisional TDI of 50ug/kgbw/day for all phthalate esters in contact with food (excluding diethylphthalate = 500ug/kgbw/day SCF (1996)).	Not stated.	Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>	<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
Health Protection Agency (HPA)	Data review	No drinking water standard or soil standard. Air standard WEL of LTEL(8 hour reference period): 0.3 ppm (5 mg m-3).	Not stated.	Plastic Materials and Articles In Contact With Food (England) Regulation 2008 look at specific limits on phthalate transfer into food. BMD are being set by COT for DEHP	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949</a>
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	Data review	Reference to a group restriction of 0.05mg/kg bw/day. Dibutylphthalate assessed further. References noted other effects but did not provide effect doses - synergistic /antagonistic effects with TCE and haptachlor, exposure of rats to high levels during pregnancy inducing a disorders in offspring similar to human Testicular Dysgenesis Syndrome, and in fetal life a substantial reduction in anogenital distances.	Not stated.	Jul 1996 'STATEMENT ON PHTHALATES IN INFANT FORMULAE' to TDIs by EC SCF . TOX/2003/09	<a href="http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf">http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf</a> also in <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> referring to SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a> . (Other sites with no dose data <a href="http://cot.food.gov.uk/pdfs/reportindexed.pdf">http://cot.food.gov.uk/pdfs/reportindexed.pdf</a> <a href="http://cot.food.gov.uk/pdfs/vutreportmarch2007.pdf">http://cot.food.gov.uk/pdfs/vutreportmarch2007.pdf</a> , <a href="http://cot.food.gov.uk/pdfs/2003-09endocrine.PDF">http://cot.food.gov.uk/pdfs/2003-09endocrine.PDF</a> , <a href="http://cot.food.gov.uk/pdfs/cotsection06.pdf">http://cot.food.gov.uk/pdfs/cotsection06.pdf</a> , <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a> , <a href="http://cot.food.gov.uk/pdfs/reportindexed.pdf">http://cot.food.gov.uk/pdfs/reportindexed.pdf</a> )
Expert Panel on Air Quality Standards (EPAQS)	N/A	N/A	N/A	N/A	N/A
European Chemicals Bureau (ECB)	Rat - see description	Rat, F-344, males and females Diet, 2 years; GLP, comparable to guideline study.	RDT (effect on Kidneys). Both sexes: ↑ absolute and relative kidney weight. Kidney lesions more severe at highest dose.	European Union Risk Assessment Report Volume 80 , 2008	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
	Rat - see description	Rat, Sprague- Dawley, males and females Diet, 3- generation guideline study .	Testes. Testicular toxicity: increased incidences of small testes, epididymes and seminal vesicles, also minimal testes atrophy. Toxicity aggravated by exposure during gestational/pup-period .		
	Mouse - see description	Mouse, CD-1, males and females Diet, continuous breeding study; GLP, comparable to guideline study.	Fertility. Dose dependent ↓ in the number of litters and ↓ proportion of live pups; both sexes affected.		
	Rat - see description	Rat, Sprague- Dawley, males and females Diet, 3-generation guideline study.	Developmental toxicity (see testicular effects above). Toxicity aggravated by exposure during gestational/pup-period.		
European Food Safety Authority (EFSA)	Data review	Based on NOAEL of 4.8 mg/kg bw/day for testicular developmental toxicity by Wolfe and Layton (2003), considered more robust than previous studies. Notes that NOELs for reproductive performance and fertility were 340 mg/kg bw/day and for developmental toxicity 113 mg/kg bw/day. (States that TDI of 0.05 mg/kg bw set by SCF based on peroxisome proliferation in rodent liver, no longer considered relevant to humans)	Testicular toxicity and developmental toxicity	Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in Contact with Food (AFC) on a request from the Commission related to Bis(2-ethylhexyl)phthalate (DEHP) for use in food contact materials Question N° EFSA-Q-2003-191 Adopted on 23 June 2005 by written procedure	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true</a> <a href="http://www.efsa.europa.eu/EFSA/efsa_locale-1178620753812_1178620770530.htm">http://www.efsa.europa.eu/EFSA/efsa_locale-1178620753812_1178620770530.htm</a>

Bis ethylhexyl phthalate, di(2 ethylhexyl)phthalate or DEHP	CAS Number:	117-81-7		Assessor A:	Barry Mitcheson, Enviros	Assessor B:	Charlotte Clark, Hyder	Final review:	Panel/SF				
		Date	05/05/2009	Date	06/05/2009	Date	26/08/2009						
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	16 December 1994 report	07/04/2009	TDI	0.05	mg/kgbw/day	50	Not given (but note the basis of peroxisomal proliferation now not regarded as significant in humans)	NOEL of peroxysomal proliferation	5	NOEL mg/kg/bw/d	100	Not given but less than 100 considered
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>		07/04/2009	No data on non-carcinogenicity - see description	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/jecfa/en/">http://who.int/ipcs/food/jecfa/en/</a>		07/04/2009	DEHP use lowest Level attainable (1988)	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2006	08/04/2009	WHO for Drinking Water standard of 8ug/l	25	ug/kg of body weight for DEHP,	25	Low	Based on a NOAEL for peroxisomal proliferation in the liver in rats.	2.5	NOAEL mg/kg/bw/d	100	Inter- and Intraspecies variation
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009	TDI	4	ug/kg bw/day	4	Very low superseded by EFSA. Low confidence in study also expressed by others.	Testicular effects	3.7	mg/kg bw /day	1000	10 for extrapolation to life time, 10 for intra-species and 10 for inter-species variation
	Other values detailed in study	1993	20/04/2009	TDI	20	ug/kg bw/day	20	Very low.	NOAEL	19	mg/kg bw/day	1000	Not stated
		1997	20/04/2009	TDI	50	ug/kg bw/day	50	Very low.	Not stated.	Not stated.	Not stated.	N/A	N/A
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	19/04/2007	08/04/2009	44ug/kgbw/day based on developmental studies by Wolkowski-Tyl et al.	0.044	mg/kgbw/day	44	No t given	NOEL for non-hepatic peroxisome proliferation effects.	44	mg/kg/day	1000	10 for inter-species variation, 10 for intra-species variation and 10 for potential teratogenicity
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	08/04/2009	TDI Oral	0.1 mg/kg/day/ 0.06 mg/kg/day	Int. / Chronic		100 / 100	Repro. / Repro.	Final			Both values = 10 for animals to humans, 10 for human variability.
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Last updated on Thursda	08/04/2009	Reference to IRIS									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	05/01/1991 last note in	08/04/2009	Reference Dose	0.02	mg/kg bw/day	20	Medium	Increased relative liver weight LOAEL: 0.04% of diet (19 mg/kg bw/day)	19	mg/kg bw /day	1000	10 for inter-species variation and 10 for sensitive humans. Additional factor of 10 as guinea pig exposure longer than subchronic but less than lifetime, LOAEL effect was considered minimally adverse.
Entrez PubMed	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">http://www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>	Date of paper 2005 (abstract only)	20/04/2009	TDI	37	ug/kg bw/day	37						
		Date of paper 2003 (abstract only)	20/04/2009	TDI	37	ug/kg bw/day	37						
		Date of paper 2006 (abstract only)	20/04/2009	RfD	20	ug/kg/day	20						
		Date of paper 2006 (abstract only)	20/04/2009	TDI	20-48	ug/kg bw/day	range 20-48						

Bis ethylhexyl phthalate,  
di(2 ethylhexyl)phthalate or DEHP

Scientific Committee on Food (SCF) pre 2002	Data review	Based on peroxysomal proliferation. Also refers to NOEL of 35/mg/kg/bw/d for reproductive toxicity.	Peroxisomal proliferation	Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series.	<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_36.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_36.pdf</a>
International Agency for Research on Cancer (IARC)	Data review	Overall evaluation is not classifiable as to its carcinogenicity to humans (Group3) - this updated the previous issue of 1982 - mechanism that increases the incidence of tumours in rats and mice is not relevant to humans.	N/A	N/A	N/A
Joint Expert Committee on Food Additives (JECFA)	N/A	N/A	N/A	N/A	N/A
WHO Guidelines for drinking water Quality	Rat	Hinton RH et al. Effects of phthalic acid esters on the liver and thyroid.	Liver	DEHP in Drinking-Water Background document for development of WHO Guidelines for Drinking-water Quality WHO 2003, & Guidelines for Drinking-water Quality FIRST ADDENDUM TO THIRD EDITION Volume 1 Recommendations WHO 2006.	<a href="http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf</a> & <a href="http://www.who.int/water_sanitation_health/dwq/chemicals/di2ethylhexylphthalate.pdf">http://www.who.int/water_sanitation_health/dwq/chemicals/di2ethylhexylphthalate.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Mice	Baars et al study exposure in household dust value of 4ug/kgbw/day. Also references reproduction study and teratogenicity studies. Oral NOAEL 35mg/kg bw/day for reproductive effects noted. Most prominent effects in repeated dose study are testicular - dietary NOAEL of 3.7 mg/kg bw/day for 13 weeks.	Testes	Re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
	Not stated	Not stated	Not stated	Hassauer M et al, (1993) Basisdate Toxikologie fur umweltrelevante Stoffe zur Gefahrenbeurteilung bei Altlasten, Germany	
	Not stated	Not stated	Not stated	EC (1997) Food Sciences and Techniques, Report of the Scientific Committee for Food, no.39, Office of Official Publications of the European Communities, Luxembourg.	
Health Canada Toxicological Values	Reproduction toxicity in mice	Wolkowski-Tyl et al. (1984a) mouse study found LOAEL for mothers and offspring was 91 mg/kg bw/d (maternal toxicity, increased resorptions and dead foetuses) NOEL for mothers and offspring was 44 mg/kg bw/d - teratogenic effects at higher doses and evidence of teratogenicity Shiota and Mima study (1985). Data indicate humans may be less sensitive than rodents but insufficient information to take this into account when setting UF.	44 mg/[kg (b.w.)·d] is the NOEL for effects other than those related to hepatic peroxisome proliferation [i.e., adverse developmental effects observed at the next highest dose in the investigation by Wolkowski-Tyl et al. (1984a); lower NOELs in other developmental studies are a function predominantly of wider spacing of the administered doses].	Bis(2-ethylhexyl) Phthalate - PLS1. Canadian Environmental Protection Act Priority Substances List Assessment Report Bis(2-ethylhexyl)Phthalate 1994. Study for NOEL is Wolkowski-Tyl R, C.Jones Price, MC Marr and CA Kinmel Teratologic Evaluation of Diethylhexyl Phthalate in CD-1 Mice, Final Report, National Center for Toxicological Research, Jefferson, AR, PB5-15674 (1984)	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-isp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-isp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Rat	Male and female rats fed DEHP for 104 weeks. NOAEL for females of 7.3mg/kg/day.	For Intermediate the lowest dose, 14 mg/kg/day, is a NOAEL for reproductive toxicity in the male and female mice. For Chronic the lowest dose, 5.8 mg/kg/day, is a NOAEL for testicular toxicity in the male rats.	Toxicological Profile for Di (2 ethylhexyl) Phthalate, September 2002 Study from David RM, Moore MR, Finney DC, et al. 2000a. Chronic toxicity of di(2-ethylhexyl)phthalate in rats. Toxicol Sci 55:433-443.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a> (& <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)
USEPA Health Advisors					
USEPA Integrated Risk Information System (IRIS)	See Description	Increased relative liver weight  Guinea Pig Sub-chronic-to-Chronic Oral Bioassay	Increased relative liver weight. Guinea Pig sub-chronic-to-chronic oral Bioassay. Carpenter et al., 1953	IRIS Database Carpenter CP, CS Weil and HF Smyth 1953 Chronic oral toxicity of di(2 ethyl hexyl)phthalate for rats and guinea pigs. Arch. Indust. Hyg. Occup. Med. 8: 219-226	<a href="http://www.epa.gov/ncea/iris/subst/0014.htm">http://www.epa.gov/ncea/iris/subst/0014.htm</a>
Entrez PubMed		level established by the EU Scientific Committee for Toxicity, Ecotoxicity and Environment (SCTEE)		Human monitoring of phthalates and risk assessment. 1: J Toxicol Environ Health A. 2005 Aug 27;68(16):1379-92.	<a href="http://www.ncbi.nlm.nih.gov/pubmed/16009652?ordinalpos=3&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/16009652?ordinalpos=3&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>
		level established by the EU Scientific Committee for Toxicity, Ecotoxicity and Environment (SCTEE)		An estimation of the daily intake of di(2-ethylhexyl)phthalate (DEHP) and other phthalates in the general population. Int J Hyg Environ Health. 2003 Mar;206(2):77-83	<a href="http://www.ncbi.nlm.nih.gov/pubmed/12708228?ordinalpos=2&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/12708228?ordinalpos=2&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>
		no referece - likely to be USEPA		Di(2-ethylhexyl)phthalate (DEHP): human metabolism and internal exposure--an update and latest results Int J Androl. 2006 Feb;29(1):155-65; discussion 181-5	<a href="http://www.ncbi.nlm.nih.gov/pubmed/16466535?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdbfrom=pubmed">http://www.ncbi.nlm.nih.gov/pubmed/16466535?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdbfrom=pubmed</a>
		no reference		Di(2-ethylhexyl)phthalate (DEHP): human metabolism and internal exposure--an update and latest results. Int J Androl. 2006 Feb;29(1):155-65; discussion 181-5	<a href="http://www.ncbi.nlm.nih.gov/pubmed/16466535?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdbfrom=pubmed">http://www.ncbi.nlm.nih.gov/pubmed/16466535?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdbfrom=pubmed</a>

Bis ethylhexyl phthalate, di(2 ethylhexyl)phthalate or DEHP		CAS Number:	117-81-7	Assessor A:	Barry Mitcheson, Enviro	Assessor B:	Charlotte Clark, Hyder	Final review:	Panel/SF				
		Date	05/05/2009	Date	06/05/2009	Date	26/08/2009						
TDI inhal				Recommended TDI inhal	Units	Justification							
					ug.kg-1.d-1	Insufficient data with sufficient detail on derivation to derive							
Organisation		Last Updated		Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>	11-Sep-08	31/03/2009										
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>		06/04/2009	WEL & STEL	8 hrs - 5, 15 mins - 10	mg.m-3							
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search : 2005 Review of report by MS Technical Experts finalised: September 2005 Final report: 2008	07/04/2009	Data for Oral also applied to dermal an inhalation in risk assessment. NOAEL for kidneys (14.5mg/kgbw/day), testicular (4.8mg/kgbw/day, reproduction (10mg/kgbw/day) development 4.8mg/kgbw/day) and added a MOS of 30 to 250 for adults to babies and 100 for children	0.145	mg/kgbw/day	145	Not given	Moore (1996) with adjustment for 50% absorption	14.5	NOAEL mg/kgbw/day	100	An assessment factor of 10 is used for potential species differences. Assessment factors of 3 and 10 are used for potential intraspecies differences for the worker and general population, respectively. Giving Margin of Safety of 30 (commercial) to 100 for children. We have used the 100 figure. For infants of 3- 12 month a factor of 20 and for <3 months a factor of 250 was considered but it was noted that " all member states do not agree that newborns/infants need a higher margin of safety in this particular case".)
					0.048	mg/kgbw/day	48	Not given	Wolfe et al. (2003) Oral exposure	4.8	NOAEL mg/kgbw/day		
					0.1	mg/kgbw/day	100	Not given	Lamb et al. (1987) with adjustment for 50% absorption	10	NOAEL mg/kgbw/day		
					0.048	mg/kgbw/day	48	Not given	Wolfe et al. (2003) Oral exposure	4.8	NOAEL mg/kgbw/day		
IPCS INCHEM	<a href="http://inchem.org/">http://inchem.org/</a>		07/04/2009	occupational exposure limits	5 (TLV), 10 (MAC)	mg/m3							
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>		08/04/2009	Guideline value	120	ug/m3	34.2						
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009										
					1993	20/04/2009	exposure limit	0.7	ug/m3			NOAEC	1.4
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	08/04/2009										
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Last updated on Thursday	08/04/2009	Reference to IRIS									
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	1998	21/04/2009	Occupational Health values - OSHA	5	mg/m3 (TWA)							
					5	mg/m3							
					5	mg/m3 (10hr TWA)							

Bis ethylhexyl phthalate,  
di(2 ethylhexyl)phthalate or DEHP

TDI inhal					
Organisation	Study type	Description	Response	Reference	Web link
Health Protection Agency (HPA)		Page on exposure standards details no drinking water standard no soil standard or air standard WEL of LTEL(8 hour reference period): 0.3 ppm (5 mg m <sup>-3</sup> )		Phthalates (Diisononylphthalate and Di(2-ethylhexyl)phthalate) Incident management, Health Protection Agency 2008	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949</a>
Health and Safety Executive (HSE)	Data review	HSC/04/06 Annex C All three listed. WEL 5mg/m <sup>3</sup> and STEL 10mg/m <sup>3</sup> . Risk Phrases refer to R60 and R61 (harm fertility and harm the unborn child).		EH40/2005 Table 1: List of approved workplace exposure limits (as consolidated with amendments October 2007)	<a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>
European Chemicals Bureau (ECB)	See Description	Rat, F-344, males and females Diet, 2 years; GLP, comparable to guideline study Both sexes: ↑ absolute and relative kidney weight More severe kidney lesions were observed at the highest dose level	RDT (effect on Kidneys)	European Union Risk Assessment Report Volume 80 , 2008	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
	See Description	Rat, Sprague- Dawley, males and females Diet, 3- generation guideline study Testicular toxicity as well as Developmental toxicity: increased incidences of small testes, epididymes, and seminal vesicles, as well as cases of minimal testes atrophy. The toxicity was aggravated by exposure during the gestational/pup-period	Testes		
	See Description	Mouse, CD-1, males and females Diet, continuous breeding study; GLP, comparable to guideline study Fertility ↓ (dose dependent ↓ in the number of litters) and ↓ proportion of live pups; crossover matings showed that both sexes were affected	Fertility		
	See Description	Rat, Sprague-Dawley, males and females Diet, 3- generation guideline study Testicular toxicity as well as Developmental toxicity: increased incidences of small testes, epididymes, and seminal vesicles, as well as cases of minimal testes atrophy. The toxicity was aggravated by exposure during the gestational/pup-period	Developmental effects on foetus		
IPCS INCHEM					
WHO Guidelines for drinking water Quality		Stated value - source unknown		The regulations for indoor air pollution in Japan: A public health perspective, Kenichi Azuma	<a href="http://www.euro.who.int/Document/E87878_pt3.pdf">http://www.euro.who.int/Document/E87878_pt3.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels		Baars et al states that inhalation not considered relevant due to low volatility. The dust paper uses the oral EFSA value given above		re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/200	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
	rats	systemic toxicity in rats		Hassauer M et al, (1993) Basisdate Toxikologie fur umweltrelevante Stoffe zur Gefahrenbeurteilung bei Altlasten, Germany	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels		No inhalation MRLs were derived for DEHP due to inadequate data for this route of exposure. Inhalation database for DEHP is essentially limited to two studies in rats. Systemic effects (liver weight and lung function ) intermediate study only . LOAEL = 100mg/m <sup>3</sup> , NOAEL = 50mg/m <sup>3</sup> .	Reversible effects in the lungs and liver following exposure for 28 days and no evidence for reproductive or developmental toxicity (Klimisch et al. 1991; Merkle et al. 1988).	Toxicological Profile for Di(2-ethylhexyl)phthalate (DEHP) September 2002 including Reference: David RM, Moore MR, Finney DC, et al. 2000a. Chronic toxicity of di(2-ethylhexyl)phthalate in rats. Toxicol Sci 55:433-443.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a> (& <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)
USEPA Health Advisors					
Toxicology Data Network (Toxnet)				Occupational Health Value	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+117-81-7">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+117-81-7</a>
				Occupational Health Value	-
				Occupational Health Value	-

Bis ethylhexyl phthalate, di(2 ethylhexyl)phthalate or DEHP	CAS Number:	117-81-7	Assessor A: Barry Mitcheson, Enviros	Assessor B: Charlotte Clark, Hyder	Final review: Panel/SF
			Date 05/05/2009	Date 06/05/2009	Date 26/08/2009

ID oral			Recommended ID oral	Units	Justification									
			n/a		Weight of evidence indicates not carcinogenic.									
Organisation	Last Updated		Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating					Basis	
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	<a href="http://www.advisorybodies.doh.gov.uk/coc/index.htm">http://www.advisorybodies.doh.gov.uk/coc/index.htm</a>	06/04/2009	No dose data identified. Chemicals for which a tumorigenic effect was first observed between 53 and 80 week in rats and/or mice.											
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search : 2005 Review of report by MS Technical Experts finalised: September 2005 Final report: 2008	07/04/2009											
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	2000	07/04/2009											
ICPS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>		07/04/2009											
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/en">http://www.who.int/water_sanitation_health/dwa/guidelines/en</a>	2006	08/04/2009	TDI but relates to carcinomas and hepatocarcinogenicity	25 ug/kg of body weight for DEHP, based on WHO DWS of 8ug/l. Data given as	ug/l	25	Low	Based on a NOAEL for peroxisomal proliferation in the liver in rats,	2.5	mg/kg bw/d	NOAEL mg/kg of body weight per day	100	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001	08/04/2009											
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	19/04/2007	08/04/2009											
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	08/04/2009											
USEPA Integrated Risk Information System (IRIS)	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	02/01/1993	08/04/2009	Oral Slope Factor	1.4E-2/mg/kg/day	0.000714286 mg/kgbw/day	0.714286	Medium						

Bis ethylhexyl phthalate,  
di(2 ethylhexyl)phthalate or DEHP

ID oral					
Organisation	Study type	Description	Response	Reference	Web link
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)				CC/01/25 COMMITTEE ON CARCINOGENICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT THE MINIMUM DURATION OF CARCINOGENICITY STUDIES IN RATS, November 2001	<a href="http://www.iacoc.org.uk/papers/documents/mindurcarcstudy.PDF">http://www.iacoc.org.uk/papers/documents/mindurcarcstudy.PDF</a>
European Chemicals Bureau (ECB)		Based on the overall evaluation of the studies on mutagenicity (see Section 4.1.2.8) DEHP and its major metabolites can be regarded as non-genotoxic agents.		European Union Risk Assessment Report Volume 80 , 2008	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
International Agency for Research on Cancer (IARC)		Di(2-ethylhexyl) phthalate is <i>not classifiable as to its carcinogenicity to humans (Group 3)</i> .		International Agency for Research on Cancer (IARC) - Summaries & Evaluations DI(2-ETHYLHEXYL) PHTHALATE (Group 3) VOL.: 77 (2000) (p. 41)	<a href="http://www.inchem.org/documents/iarc/vol77/77-01.html">http://www.inchem.org/documents/iarc/vol77/77-01.html</a>
ICPS Environmental Health Criteria (EHC) Monographs		No data in EHC131..." Currently there is not sufficient evidence to suggest that DEHP is a potential human carcinogen."			<a href="http://www.inchem.org/documents/ehc/ehc/ehc131.htm">http://www.inchem.org/documents/ehc/ehc/ehc131.htm</a>
WHO Guidelines for drinking water Quality			Hinton RH et al. Effects of phthalic acid esters on the liver and thyroid.	Di(2-ethylhexyl)phthalate in Drinking-water Background document for development of WHO Guidelines for Drinking-water Quality WHO 2003, & Guidelines for Drinking-water Quality FIRST ADDENDUM TO THIRD EDITION Volume 1 Recommendations WHO 2006	<a href="http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf</a> & <a href="http://www.who.int/water_sanitation_health/dwq/chemicals/di2ethylhexylphthalate.pdf">http://www.who.int/water_sanitation_health/dwq/chemicals/di2ethylhexylphthalate.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels		Baars et al states that there is no indication that DEHP is a genotoxic carcinogen.		re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/200	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Values		"The weight of evidence also indicates that the metabolites of bis(2-ethylhexyl) phthalate, mono(2-ethylhexyl) phthalate, and 2-ethylhexanol, are not genotoxic."		Bis(2-ethylhexyl) Phthalate - PLS1	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels		No studies located regarding genotoxic effects in humans . DEHP has been extensively tested in short-term genotoxicity assays with predominantly negative or false-positive results. Weight of evidence indicates that DEHP best characterized as an epigenetic toxicant.		Toxicological Profile for Di(2-ethylhexyl)phthalate (DEHP) September 2002 including Reference: David RM, Moore MR, Finney DC, et al. 2000a. Chronic toxicity of di(2-ethylhexyl)phthalate in rats. Toxicol Sci 55:433-443.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a> (& <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)
USEPA Integrated Risk Information System (IRIS)	Mouse/B6C3F1, male. Dietary.	Classification — B2; probable human carcinogen. Basis — Orally administered DEHP produced significant dose-related increases in liver tumor responses in rats and mice of both sexes. Based on risk of 1 in 1e5.	Tumor Type: hepatocellular carcinoma and adenoma	NTP, 1982 Classification	<a href="http://www.epa.gov/ncea/iris/subst/0014.htm">http://www.epa.gov/ncea/iris/subst/0014.htm</a>

Bis ethylhexyl phthalate, di(2 ethylhexyl)phthalate or DEHP	CAS Number: 117-81-7	Assessor A: Barry Mitcheson, Enviro	Assessor B: Charlotte Clark, Hyder	Final review: Panel/SF
		Date: 05/05/2009	Date: 06/05/2009	Date: 26/08/2009

ID inhal				Recommended Id inhal	Units	Justification						
				n/a		Weight of evidence indicates not carcinogenic.						
Organisation	Last Updated		Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating				Basis
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>	11-Sep-08	31/03/2009	Page on exposure standards details no drinking water standard no soil standard or air standard WEL of LTEL(8 hour reference period): 0.3 ppm (5 mg m-3 )								
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>		06/04/2009	HSC/04/06 Annex C All three listed. WEL 5mg/m3 and STEL 10mg/m3. Risk Phrases refer to R60 and R61 (harm fertility and harm the unborn child)								
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	<a href="http://www.advisorybodies.doh.gov.uk/coc/index.htm">http://www.advisorybodies.doh.gov.uk/coc/index.htm</a>		06/04/2009	No dose data identified. Chemicals for which a tumorigenic effect was first observed between 53 and 80 week in rats and/or mice.								
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search : 2005 Review of report by MS Technical Experts finalised: September 2005 Final report: 2008	07/04/2009									
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	2000	07/04/2009									
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001	08/04/2009									
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	19/04/2007	08/04/2009									
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	08/04/2009									
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Last updated on Thursday	08/04/2009									

Bis ethylhexyl phthalate,  
di(2 ethylhexyl)phthalate or DEHP

ID inhal					
Organisation	Study type	Description	Response	Reference	Web link
Health Protection Agency (HPA)				Phthalates (Diisononylphthalate and Di(2-ethylhexyl)phthalate) Incident management, Health Protection Agency 2008	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949</a>
Health and Safety Executive (HSE)					<a href="http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf">http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf</a>
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)				CC/01/25 COMMITTEE ON CARCINOGENICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT THE MINIMUM DURATION OF CARCINOGENICITY STUDIES IN RATS, November 2001	<a href="http://www.iacoc.org.uk/papers/documents/mindurcarcstudy.PDF">http://www.iacoc.org.uk/papers/documents/mindurcarcstudy.PDF</a>
European Chemicals Bureau (ECB)		Based on the overall evaluation of the studies on mutagenicity (see Section 4.1.2.8) DEHP and its major metabolites can be regarded as non-genotoxic agents.		European Union Risk Assessment Report Volume 80 , 2008	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
International Agency for Research on Cancer (IARC)		Di(2-ethylhexyl) phthalate is <i>not classifiable as to its carcinogenicity to humans (Group 3)</i> .		International Agency for Research on Cancer (IARC) - Summaries & Evaluations DI(2-ETHYLHEXYL) PHTHALATE (Group 3) VOL.: 77 (2000) (p. 41)	<a href="http://www.inchem.org/documents/iarc/vol77/77-01.html">http://www.inchem.org/documents/iarc/vol77/77-01.html</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels		Baars et al states that there is no indication that DEHP is a geotaxis carcinogen.		re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/200	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Values		"The weight of evidence also indicates that the metabolites of bis(2-ethylhexyl) phthalate, mono(2-ethylhexyl) phthalate, and 2-ethylhexanol, are not geotaxis."		Bis(2-ethylhexyl) Phthalate - PLS1	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels		No studies located regarding genotoxic effects in humans . DEHP has been extensively tested in short-term genotoxicity assays with predominantly negative or false-positive results. Weight of evidence indicates that DEHP best characterized as an epigenetic toxicant.		Toxicological Profile for Di(2-ethylhexyl)phthalate (DEHP) September 2002 including Reference: David RM, Moore MR, Finney DC, et al. 2000a. Chronic toxicity of di(2-ethylhexyl)phthalate in rats. Toxicol Sci 55:433-443.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a> (& <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)
USEPA Health Advisors				Reference to IRIS	

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MDI			Recommended MDI oral	Units	Justification: High end exposure selected by FSA from diet study in 1993. Exposure may be greater for infants due to infant milk bottles, but will be for a relatively short period. High values selected instead of Mean to allow for potential exposure from toys.		
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Food Standards Agency	1993	diet	300	ug day-1	Mean 0.15 mg/person/day and 0.3mg/person/day for high end	82: MAFF UK - Phthalates in Food (March 1996) Table 2: Estimated mean and high level (97.5th percentile) intakes of individual phthalates from carcass meat, poultry, eggs and milk, based on the analysis of 1993 Total Diet Study samples.	<a href="http://www.food.gov.uk">www.food.gov.uk</a> <a href="http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/table2.htm#Table2">http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/table2.htm#Table2</a>
	1998	Infant milk	77.28	ug day-1	At birth exposure is 13.8ug/kgbw/day, at six months 7.7ug/kgbw/day. Conversion made using 5.6kg bodyweight fo 0-1 year old.	Food Surveillance sheet Number 168 December 1998 MAFF UK - PHTHALATES IN INFANT FORMULAE - FOLLOW-UP SURVEY Concentrations and Estimated Average. Exposure to Individual and Total Phthalates of Infants at Birth and Six Months of Age from Retail Infant Formulae Table 2:	<a href="http://archive.food.gov.uk/maff/archive/food/infosheet/1998/no168/tables.htm">http://archive.food.gov.uk/maff/archive/food/infosheet/1998/no168/tables.htm</a>
Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	12/04/2009	No Data				TOX/2004/25 COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD, CONSUMER PRODUCTS AND THE ENVIRONMENT- TOXICOLOGICAL EVALUATION OF A PILOT STUDY FOR A BREAST- MILK ARCHIVE	<a href="http://www.cot.food.gov.uk">www.cot.food.gov.uk</a>
European Chemicals Bureau (ECB)	12/04/2009	Food, air and water	1036	ug day-1	14.8ug/kg bw/day for a 70kg adult based on modelling of a sewage treatment plant scenario	European Union Risk Assessment Report Volume 80 , 2008.	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a> <a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
	12/04/2009	Food, air and water	135.1	ug day-1	1.93ug/kg bw/day for a 70kg adult based on modelling	European Union Risk Assessment Report Volume 80 , 2008.	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
	12/04/2009	Food, air and water	1190	ug day-1	17ug/kg bw/day for a 70kg adult based on biomonitoring near sewage treatment works.	European Union Risk Assessment Report Volume 80 , 2008.	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
	12/04/2009	Food, air and water	664	ug day-1	83ug/kg bw/day for a 8kg child based on modelling of exposure at a sewage treatment plant	European Union Risk Assessment Report Volume 80 , 2008,	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
	12/04/2009	Food, air and water	155.2	ug day-1	19.4ug/kg bw/day for a 8kg child based on regional modelling	European Union Risk Assessment Report Volume 80 , 2008.	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
European Food Safety Authority (EFSA)	12/04/2009	Diet	0.15 (mean) 0.3 (97.5th) mg/person/day	300/150ug/day	Limited available data on DEHP in foods and diets in UK and Denmark used to estimate dietary exposure. In the UK, mean and high (97.5th percentile) dietary intakes of DEHP estimated to be respectively 0.15 and 0.3 mg/person/day in the adult population (equivalent to 2.5 and 5 µg/kg bw/day) for a 60 kg adult. Exposure of infants via formulae exposure calculated to be 23.5ug/kg be/day(Muller et al)	Opinion of the Scientific Panel on Food Additives, Flavours, Processing Aids and Materials in Contact with Food (AFC) on a request from the Commission related to Bis(2-ethylhexyl)phthalate (DEHP) for use in food contact materials Question N° EFSA-Q-2003-191 Adopted on 23 June 2005 by written procedure	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a> <a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true</a>
	12/04/2009	Diet	300 for adults, in first study and in second study 315 for adults, 208 for 1-6 children and 11 * bodyweight of a 7-14 year old child	ug day-1	A Danish study estimated mean DEHP exposure ranging from 0.19 to 0.3 mg/day, (i.e. 2.7 to 4.3 µg/kg bw/day, for 70 kg adult). Based on the highest concentration of DEHP, high percentile exposure estimated as 1.1 mg/day (i.e. 15.7 µg/kg bw/day). Another Danish dietary study apportioned exposure as leaf crops (53%), root crops (13%), milk (12%) and fish (10%). Total oral intake estimated as 4.5 µg/kg bw/day (adults), 26 µg/kg bw/day (children 1-6 years old, and 11 µg/kg bw/day (children 7-14 years old).		<a href="http://ec.europa.eu/fppd/fs/sc/scf/index_en.html">http://ec.europa.eu/fppd/fs/sc/scf/index_en.html</a>
	12/04/2009	Infant milk formula and breast milk	56 for <six months 22.4 to 131.6 for six months (note body weight assumed to be 5.6kg (possibly large for <six months)	ug day-1	Based on the detection limit, intake from infant formulae would be <10 µg/kg bw/day in infants of <6 months, and 4 µg/kg bw/day in infants of >6 months. For infants >6 months, ready-to-use baby foods also considered and exposure was therefore estimated to be 23.5 µg/kg bw/day		
European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC)	22/04/09 (1998)	daily lifetime exposure	2.3-6ug/kg bw	420 ug/day	Estimates of average daily lifetime exposure to DEHP - drinking water thought to be low but individual instances may be as high as 170ug/l (not included in value)	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Phthalate migration from soft PVC toys and child care articles Opinion expressed at the CSTEE third plenary meeting Brussels 24 April 1998.	<a href="http://www.ecetoc.org/">www.ecetoc.org/</a> <a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf</a>
	22/04/09 (2004)	estimate exposure	7.1ug/kg bw/day	497 ug/day	Calculated from urinary excretion of DEHP metabolites	Scientific Committee on toxicity, Ecotoxicity and the Environment (CSTEE) Opinion on the results of the Risk Assessment of: Bis(2 ethylhexyl)phthalate (DEHP) Human Health Part . Adopted by the CTSEE during the 41th plenary meeting of 8 January 2004	<a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out214_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out214_en.pdf</a>
International Agency for Research on Cancer (IARC)	12/04/2009	Background data insufficient to give MDI			The highest levels of DEHP in foods are found in milk products, meat and fish and in other products with a high fat content, where concentrations up to 10 mg/kg have been reported	Volume 77 2000 IARC International Agency for Research on Cancer (IARC) - Summaries & Evaluations	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a> <a href="http://inchem.org/documents/iarc/vol77/77-01.html">http://inchem.org/documents/iarc/vol77/77-01.html</a>

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IPCS Environmental Health Criteria (EHC) Monographs	12/04/2009	Food	300-2000 (US) and <20ug/day in UK (1987)	20ug/day	Based on food analysis, average exposure in the USA estimated at around 0.3 mg/person/day and maximum 2 mg/person per day. Survey of plasticizer levels in food-contact material and food, by MAFF (1987) stated that DEHP has very limited use in food-contact material, and the maximum intake from food sources was estimated at 20 mg/person/day.	International Programme of Chemical Safety. Environmental Health Criteria 131 Diethylhexyl phthalate WHO 1992	<a href="http://incchem.org/pages/ehc.html">http://incchem.org/pages/ehc.html</a> . ENVIRONMENTAL HEALTH CRITERIA 131 -DIETHYLHEXYL PHTHALATE (1992) <a href="http://www.inchem.org/documents/ehc/ehc/ehc131.htm">http://www.inchem.org/documents/ehc/ehc/ehc131.htm</a>
Joint Expert Committee on Food Additives (JEFCA)	12/04/2009					INCHEM - BIS (2-ETHYLHEXYL)PHTHALATE	<a href="http://www.who.int/ipcs/food/jefca/en/">www.who.int/ipcs/food/jefca/en/</a>
WHO Guidelines for Drinking Water Quality	12/04/2009	Food	About 200 ug/day mostly from food	200ug/day	Water: In Japan, DEHP was in the range 0.6–3.2 µg/litre. DEHP in tapwater in two US cities approximately 1 µg/litre and in Japan at levels in the range of 1.2–1.8 µg/litre. In “finished” drinking-water in 2 US cities, average of 0.05–11 µg/litre; in several major eastern cities in the USA, average levels were below 1 µg/litre. Up to 30 µg/litre reported in older surveys (1975). Food: In USA most fish contained < 0.2 mg/kg. Highest levels were in milk (31.4 mg/litre, fat basis) and cheese (35 mg/kg, fat basis). Very little migration occurs in bottles with DEHP plasticized PVC seals; all concentrations were < 0.1 mg/kg, vast majority <0.02 mg/kg. Draught beer contained <0.01–0.04 mg/kg DEHP. Individual exposure varies due to variety of products containing DEHP. Estimated average adult dose from commodities likely to be contaminated (e.g. milk, cheese, margarine) is about 200 µg/d. Exposure from air negligible compared with diet (e.g. when the concentration in city air is 50 ng/m <sup>3</sup> , the daily exposure will be less than 1 µg). The Netherlands standard for the migration of DEHP from blood containers is 10 mg of DEHP per 100 ml of ethanol.	Di(2-ethylhexyl)phthalate in Drinking-water Background document for development of WHO Guidelines for Drinking-water Quality WHO 2003, & Guidelines for Drinking-water Quality FIRST ADDENDUM TO THIRD EDITION Volume 1 Recommendations WHO 2006	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">www.who.int/water_sanitation_health/dwg/guidelines/en</a> <a href="http://www.who.int/water_sanitation_health/dwg/gdwg0506.pdf">http://www.who.int/water_sanitation_health/dwg/gdwg0506.pdf</a> & <a href="http://www.who.int/water_sanitation_health/dwg/chemicals/di2ethylhexyphthalate.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/di2ethylhexyphthalate.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	12/04/2009	All media primarily food	Dust report gives 210 to 1120 for adults and about 120 to 260ug/day for children. MPR report equated to 350 - 630ug/day for adults	ug day-1	Dust report gives Background value of DEHP for adults 3-16 µg/kg/day and for children 12-26 µg/kg/day. MPR report cites WHO guideline of 200ug/day. Gives overall uptake for phthalates as 5-9ug/kgbw/day based on addition of WHO DWS information for DEHP plus CICAD information for Butyl benzyl phthalate	Re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a> <a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Reference Values	12/04/2009	All media primarily food	5.8ug/kg/day (equivalent to 406ug/day in adult to 19.0 µg/[kg (b.w.)·d] in children equivalent to 152ug/day	ug/day	Data from table hard to interpret as food data looks incorrect (suspect that drinking water and food rows are reversed)	2007-04-19 Bis(2-ethylhexyl) Phthalate - PLS1	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a> <a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	12/04/2009	All media including occupational exposure in the uS	210 to 2100ug/day	ug day-1	Exposure to DEHP is via oral, dermal, and inhalation routes. Total daily exposure to DEHP in US is 0.21 to 2.1 mg/day (David 2000; Doull et al. 1999; Huber et al. 1996; Kohn et al. 2000; Tickner et al. 2001). Based on a 70kg adult. Principal route is oral. Water and inhalation are not considered significant. Some recent studies suggest	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a>	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
Toxicological Data Network (TOXNET)	12/04/2009	Water	0.08 to 60 ug	ug day-1	WATER INTAKE (assume 0.04 to 30 ppb)(3,4)- 0.08 to 60 ug. (SRC)	[(1) Bove JL et al; Int J Environ Anal Chem 5: 189 (1978) (2) Thuren A, Larsson P; Environ Sci Technol 24: 554-9 (1990) (3) Storm DL; pp. 67-124 in Water Contamination and Health, Wang RGM ed, NY,NY: Marcel Dekker, Inc (1994) (4) Keith LH et al; Ident and Anal of Organ Pollut in Water. Ann Arbor MI: Ann Arbor Press p 329-73 (1976)]**PEER REVIEWED**	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
Entrez PubMed	20/04/2009 Abstract of paper only (2007)	food	2.4ug/kg bw	168ug/day (assumes 70kg bw)	Average daily intake - calculated from analysis of urine samples	Intake of phthalates and di(2-ethylhexyl)adipate: results of the Integrated Exposure Assessment Survey based on duplicate diet samples and biomonitoring data. Environ Int. 2007 Nov;33(8):1012-20. Epub 2007 Jul 3	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">www.ncbi.nlm.nih.gov/entrez/query.fcgi</a> <a href="http://www.ncbi.nlm.nih.gov/pubmed/17610953?ordinalpos=7&amp;itool=EntrezSystem2.PEntrez.Pubmed.PubMed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/17610953?ordinalpos=7&amp;itool=EntrezSystem2.PEntrez.Pubmed.PubMed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>

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	20/04/2009 Abstract of paper only (2003)	median intake	13.8ug/kg bw/day	966ug/day (assumes 70kg bw)	Based on analysed urine samples from general german population	An estimation of the daily intake of di(2-ethylhexyl)phthalate (DEHP) and other phthalates in the general population. Int J Hyg Environ Health. 2003 Mar;206(2):77-83	<a href="http://www.ncbi.nlm.nih.gov/pubmed/12708228?ordinalpos=6&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/12708228?ordinalpos=6&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>
	20/04/2009 Abstract of paper only (2008)	median intake	2.7ug/kg bw/day	189ug/day (assumes 70kg bw)	Based on urine analysis of 102 german subjects	Phthalates: metabolism and exposure. Int J Androl. 2008 Apr;31(2):131-8. Epub 2007 Dec 7	<a href="http://www.ncbi.nlm.nih.gov/pubmed/18070048?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdfrom=pubmed">http://www.ncbi.nlm.nih.gov/pubmed/18070048?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdfrom=pubmed</a>
	20/04/2009 Abstract of paper only (2006)	daily intake	21ug/kg bw/day	1750ug/day (assumes 70kg bw)	General population 95th percentile value. Children value is 25ug/kg bw/day	Di(2-ethylhexyl)phthalate (DEHP): human metabolism and internal exposure - an update and latest results. Int J Androl. 2006 Feb;29(1):155-65; discussion 181-5.	<a href="http://www.ncbi.nlm.nih.gov/pubmed/16466535?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdfrom=pubmed">http://www.ncbi.nlm.nih.gov/pubmed/16466535?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DiscoveryPanel.Pubmed_Discovery_RA&amp;linkpos=5&amp;log\$=relatedreviews&amp;logdfrom=pubmed</a>
<b>MDI</b>			<b>Recommended MDIinh</b>	<b>Units</b>	<b>Justification: Value selected by ECB for adult exposure indoors, WHO has advised that exposure in cities typically less than 1ug/d therefore other inhalation sources not considered.</b>		
			<b>15</b>	<b>ug day-1</b>			
<b>Organisation</b>	<b>Date</b>	<b>Media</b>	<b>Value</b>	<b>Units</b>	<b>Description</b>	<b>Reference</b>	<b>Web link</b>
European Chemicals Bureau (ECB)	12/04/2009	Indoor air exposure		15.4ug/day	"Indoor air" (building materials) 4.4ug/kgbw/day based on concentration of 0.021mg/m3 for a 70kg adult inhaling 20m3	European Union Risk Assessment Report Volume 80 , 2008, <a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>
	12/04/2009	Indoor air exposure		19.3ug/day	"Indoor air" (building materials) 22.4ug/kgbw/day based on concentration of 0.021mg/m3 for an 8kg adult inhaling 9.3m3	European Union Risk Assessment Report Volume 80 , 2008, <a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>	
European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC)	22/04/09 (1998)	indoor air	50ug/m3	100ug/day	value for indoor air. Value for city air stated as 5-132ng/m3 which is low compared to indoor air.	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Phthalate migration from soft PVC toys and child care articles Opinion expressed at the CSTEE third plenary meeting Brussels 24 April 1998. <a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf</a>	<a href="http://www.ecetoc.org/">www.ecetoc.org/</a>
	22/04/09 (2004)	indoor air exposure for children	22ug/kg bw/day	1540ug/day	value based on concentration of 5.3ug/m3 at saturated vapour pressure. Has been x3 to account for DEHP bound to particles arriving at a total air concentration of 21.2ug/m3. Using this conc gives 424ug/day based on 20m3/day	Scientific Committee on toxicity, Ecotoxicity and the Environment (CSTEE) Opinion on the results of the Risk Assessment of: Bis(2 ethylhexyl)phthalate (DEHP) Human Health Part . Adopted by the CTSEE during the 41th penary meeting of 8 January 2004 <a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out214_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out214_en.pdf</a>	
International Agency for Research on Cancer (IARC)	12/04/2009	Ambient air limit	<2ug/day for an adult and <1ug/day for a child	ug day-1	Di(2-ethylhexyl) phthalate is ubiquitous in the general environment as a result of its widespread use in poly(vinyl chloride) products. It is found in ambient air at levels usually below 100 ng/m <sup>3</sup> .	Volume 77 2000 IARC International Agency for Research on Cancer (IARC) - Summaries & Evaluations, <a href="http://inchem.org/documents/iarc/vol77/77-01.html">http://inchem.org/documents/iarc/vol77/77-01.html</a>	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>
IPCS Environmental Health Criteria (EHC) Monographs	12/04/2009	Air	5ng/m3 (in great Lakes and Pacific) is equivalent to 0.1 ug/day, 28.6ng/m3 (in New York) is equivalent to 0.7ug/day . Levels in polluted air (up to 790ng/m3) equivalent to up to 15.8ug/day	ug day-1	In North Atlantic, Gulf of Mexico and North Pacific DEHP ranged from <LOD to 4.1ng/m3, in New York City up to 28.6ng/m3 detected. Between 0.5 and 5 ng/m3 found in the Great Lakes ecosystem and in the Swedish atmosphere. In Denmark levels were 29-132 ng/m3 , Belgium = 126 ng/m3 in polluted air, in Canada = 300 ng/m3 in polluted air, Japan = 38-790 ng/m3.	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a> <a href="http://www.inchem.org/documents/ehc/ehc/ehc131.htm">http://www.inchem.org/documents/ehc/ehc/ehc131.htm</a>	
WHO Guidelines for Drinking Water Quality	08/04/2009	Air	When the concentration in city air is 50 ng/m3, the exposure will be less than 1 µg/day	ug day-1	In ocean air DEHP was 0.4 ng/m3 to 2.9 ng/m3. In city air, phthalates in atmospheric particulates were 5 to 132 ng/m3, but 300 ng/m3 reported near municipal incinerator. Inside houses, concentration increases with temperature but decreases with humidity; after 4 months, the concentration will be about 0.05 mg/m3 (5). Exposure from air is negligible compared with that associated with food. Patients undergoing kidney dialysis may be exposed to up to 90 mg per treatment. Exposure also occurs during the transfusion of stored whole blood.	Di(2-ethylhexyl)phthalate in Drinking-water Background document for development of WHO Guidelines for Drinking-water Quality WHO 2003, & Guidelines for Drinking-water Quality FIRST ADDENDUM TO THIRD EDITION Volume 1 Recommendations WHO 2006	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">www.who.int/water_sanitation_health/dwg/guidelines/en</a> <a href="http://www.who.int/water_sanitation_health/dwg/gdwg0506.pdf">http://www.who.int/water_sanitation_health/dwg/gdwg0506.pdf</a> & <a href="http://www.who.int/water_sanitation_health/dwg/chemicals/di2ethylhexylphthalate.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/di2ethylhexylphthalate.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	12/04/2009	Background exposure. Dust report does not separate out the inhalation of indoor dust as it is small compared to	5-9ug/kg bw/day	630ug/day (using 9 and assuming 70kg)	Based on sum of DEHP and BBP.	Re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander <a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>

Bis(2 ethylhexyl)phthalate	CAS 117-81-7	Assessor A:	Barry Mitcheson, Enviros	Assessor B:	Charlotte Clark, Hyder	Final review:	Panel/SF
		Date	06/05/2009	Date	06/05/2009	Date	26/08/2009

Health Canada Toxicological Reference Values	2007 (checked 12/4/9)	Ambient and indoor air	In ambient urban air 0.0003ug/kg/day (equivalent to 0.021ug/day in adult to 0.0003 µg/[kg (b.w.)-d] in children equivalent to 0.0024ug/day. In indoor urban air 0.06ug/kg/day (equivalent to 4.2ug/day in adult to 0.18 µg/[kg (b.w.)-d] in children equivalent to 1.44ug/day.	ug/day	Data from table hard to interpret as food data looks incorrect (suspect that drinking water and food rows are reversed).	2007-04-19 Bis(2-ethylhexyl) Phthalate - PLS1	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a> <a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	12/04/2009	Difficult to extrapolate indoor air concentrations			Wide range quoted including for new PVC flooring and walls at different temperature. Data difficult to extrapolate for exposure	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a>	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
Toxicological Data Network (TOXNET)	12/04/2009	Air	Equivalent to 0.08 to 0.28ug/day based on 20m3/day	ug day-1	HSDB database AIR INTAKE (assume 0.39 to 14 ng/cm <sup>3</sup> )(1,2) - 7.8 to 280 ng;	[[1] Bove JL et al; Int J Environ Anal Chem 5: 189 (1978) (2) Thuren A, Larsson P; Environ Sci Technol 24: 554-9 (1990) (3) Storm DL; pp. 67-124 in Water Contamination and Health, Wang RGM ed, NY,NY: Marcel Dekker, Inc (1994) (4) Keith LH et al; Ident and Anal of Organ Pollut in Water. Ann Arbor MI: Ann Arbor Press p 329-73 (1976)]**PEER REVIEWED**	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
Entrez PubMed					Only daily intake values found - detailed above		<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>



<b>Bromobenzene</b>	<b>CAS Number:</b>	<b>108-86-1</b>	Assessor A: Simon Clennell-Jones (WSP)	Assessor B: David Gallagher (ERM)	Final review: Panel/SF	
	Date	19/05/2009	Date	20/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Unclassified by IARC or USEPA. Toxicological data suggests it is unlikely to be a carcinogen - TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		Unclassified by IARC or USEPA. Toxicological data suggests it is unlikely to be a carcinogen- TDlinh applied to inhalation routes
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	24	µg/kg.bw/day	USEPA PPRTV which is also the reference used by PRG region 9 and RAIS. More recent draft US EPA toxicological review for bromobenzene gives lower draft RfD but this has not been used due to DRAFT status.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	12/05/2009	12/05/2009										
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	<a href="http://www.advisorybodies.doh.gov.uk/coc/index.htm">http://www.advisorybodies.doh.gov.uk/coc/index.htm</a>	NR	12/05/2009										
Committee on the Mutagenicity of Chemicals in Food, Consumer Products and the Environment (COM)	<a href="http://www.advisorybodies.doh.gov.uk/com">http://www.advisorybodies.doh.gov.uk/com</a>	NR	12/05/2009										
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	NR	12/05/2009										
Committee on the Medical Effects of Air Pollutants (COMEAP)	<a href="http://www.advisorybodies.doh.gov.uk/comeap/index.htm">http://www.advisorybodies.doh.gov.uk/comeap/index.htm</a>	17/10/2008	12/05/2009										
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	NR	12/05/2009										
IPCS INCHEM	<a href="http://inchem.org/">http://inchem.org/</a>	NR	13/05/2009										
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	NR	13/05/2009										

## Bromobenzene

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Food Standards Agency (FSA)	rats	Dosing of bromobenzene to give rise to overt liver toxicity.	liver toxicity	Hiejne WHM et al Toxicogenomics of bromobenzene hepatotoxicity: combined transcriptomics and proteomics approach. Biochemical Pharmacology, 65, 857-875, 2003.	<a href="http://cot.food.gov.uk/pdfs/TOX-2004-02annexes.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-02annexes.pdf</a>
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	rats		liver toxicity (no definite conclusions drawn in the study). NOTE, DRAFT PAPER ONLY FOR DISCUSSION.	COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT (COT)	<a href="http://www.iacoc.org.uk/papers/documents/cc046.pdf">http://www.iacoc.org.uk/papers/documents/cc046.pdf</a>
Committee on the Mutagenicity of Chemicals in Food, Consumer Products and the Environment (COM)	rats		liver toxicity (no definite conclusions drawn in the study). NOTE, DRAFT PAPER ONLY FOR DISCUSSION.	COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT (COT)	<a href="http://www.iacom.org.uk/papers/documents/mut041_000.pdf">http://www.iacom.org.uk/papers/documents/mut041_000.pdf</a>
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	rats	dose of bromobenzene designed to elicit hepatotoxicity in rats	liver	COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT	<a href="http://cot.food.gov.uk/pdfs/TOX-2004-02.PDF">http://cot.food.gov.uk/pdfs/TOX-2004-02.PDF</a>
Committee on the Medical Effects of Air Pollutants (COMEAP)	rats		liver toxicity (no definite conclusions drawn in the study). NOTE, DRAFT PAPER ONLY FOR DISCUSSION.	COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT (COT)	<a href="http://www.advisorybodies.doh.gov.uk/pdfs/cc046.pdf">http://www.advisorybodies.doh.gov.uk/pdfs/cc046.pdf</a>
International Agency for Research on Cancer (IARC)	rats	Study of nephrotoxicity of 2-BP, a metabolite of bromobenzene.	kidney		<a href="http://www.inchem.org/documents/cicads/cicads/cicad66.htm">http://www.inchem.org/documents/cicads/cicads/cicad66.htm</a>
	mice and rats		bronchiolar neurosis	REID, W. D., HETT, K. F., HIK, J. M., & KRISHNA, G. (1973) Metabolism and binding of aromatic hydrocarbons in the lung. Am. Rev. Resp. Dis., 107: 539-551.	<a href="http://www.inchem.org/documents/ehc/ehc/ehc006.htm">http://www.inchem.org/documents/ehc/ehc/ehc006.htm</a>
IPCS INCHEM	rats	Study of nephrotoxicity of 2-BP, a metabolite of bromobenzene.	kidney	2,4,6-TRIBROMOPHENOL AND OTHER SIMPLE BROMINATED PHENOLS. First draft prepared by Mr P.D. Howe, Dr S. Dobson, and Mr H.M. Malcolm, Centre for Ecology & Hydrology, Monks Wood, United Kingdom.	<a href="http://www.inchem.org/documents/cicads/cicads/cicad66.htm">http://www.inchem.org/documents/cicads/cicads/cicad66.htm</a>
	mice and rats			JOLLOU, P. J., MITCHELL, J. R., ZAMPOGLIONE, N., & GILLETTE, J. R. (1974) Bromobenzene-induced liver necrosis: protective role of glutathione and evidence for 3,4-bromobenzene oxide as the hepatotoxic metabolite. Pharmacology, 11: 151-169.	<a href="http://www.inchem.org/documents/ehc/ehc/ehc006.htm">http://www.inchem.org/documents/ehc/ehc/ehc006.htm</a>
IPCS concise International Chemical Assessment Documents (CICADs)	rats	Study of nephrotoxicity of 2-BP, a metabolite of bromobenzene.	kidney	2,4,6-TRIBROMOPHENOL AND OTHER SIMPLE BROMINATED PHENOLS. First draft prepared by Mr P.D. Howe, Dr S. Dobson, and Mr H.M. Malcolm, Centre for Ecology & Hydrology, Monks Wood, United Kingdom.	<a href="http://www.inchem.org/documents/cicads/cicads/cicad66.htm">http://www.inchem.org/documents/cicads/cicads/cicad66.htm</a>
		hepatotoxicity of bromobenzene and bronchiolar neurosis	liver and bronchiolar neurosis		

Bromobenzene		CAS Number:	108-86-1	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	David Gallagher (ERM)	Final review:	Panel/SF			
				Date	19/05/2009	Date	20/05/2009	Date	28/08/2009			
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/iecf/en/">http://who.int/ipcs/food/iecf/en/</a>	NR	13/05/2009									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	14/06/2007	13/05/2009	Draft RfD (not to be quoted or cited)	0.006 mg.kg-1.d-1	6		BMDL10 (benchmark dose)	17.8 (adjusted to account for daily exposure)	mg/kg/bw/day	3000	10 for interspecies extrapolation, 10 for inter-individual human variability, 10 for database deficiencies and 3 for extrapolation from a sub-chronic to chronic exposure study
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	26/07/2001	NA	RfD PPRTV	0.024 mg/kg/bw/day	24	low	NOAEL	71.4	mg/kg/bw/day (duration adjusted NOAEL)	3000	10 - Interspecies variation 10 - Sub Chronic to Chronic 10 - Intraspecies variation 3 - Database deficiencies
PRG region 9	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>	Oct-04	18/05/2009	RfD PPRTV	0.02 provisional peer reviewed toxicity value (mg.kg-1.d-1)	20	unknown	unknown				
The Risk Assessment Information System	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem">http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem</a>	06/04/2009	18/05/2009	RfD PPRTV	0.02 provisional peer reviewed toxicity value (mg.kg-1.d-1)	20	low	NOAEL	unknown		3000	unknown
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppls.html</a>	26/03/2009	20/05/2009	RfD	0.02 mg/kg/bw/day	20	unknown	unknown				

TDI inhal	Recommended TDIinhal	Units	Justification
	3.43	µg/kg.bw/day	USEPA PPRTV which is also the reference used by PRG region 9 and RAIS. More recent draft US EPA toxicological review for bromobenzene gives higher draft RFC but this has not been used due to DRAFT status.

Organisation	Last Updated	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	11/05/2009	12/05/2009								
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	14/06/2007	13/05/2009	Draft RfC	0.06 mg.m-3	17.14		BMCL10HEC (benchmark concentration)	63 mg/m3	1000	10- database deficiencies 10- Interindividual variation 3- Interspecies variation 3- Sub Chronic to Chronic
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	26/07/2001	NA	RfC PPRTV	0.012 mg/m <sup>3</sup>	3.43	Low	NOAEL	34.5 mg/m3 (duration adjusted NOAEL)	3000	3 - Interspecies variation 10 - Sub Chronic to Chronic 10 - Interindividual variation 10 - Database deficiencies
PRG region 9	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>	Oct-04	18/05/2009	RfC PPRTV	0.0029 provisional peer reviewed toxicity value (mg.kg-1.d-1)	2.9	unknown	unknown			
The Risk Assessment Information System	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem">http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem</a>	06/04/2009	18/05/2009	RfC PPRTV	0.01 provisional peer reviewed toxicity value (mg.m-3)	2.86	low	NOAEL	unknown	3000	unknown
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppls.html</a>	26/03/2009	20/05/2009	RfC	0.01 mg/m <sup>3</sup>	2.86	unknown	unknown			

## Bromobenzene

Joint Expert Committee on Food Additives (JECFA)		Study of nephrotoxicity of 2-BP, a metabolite of bromobenzene.	kidney	2,4,6-TRIBROMOPHENOL AND OTHER SIMPLE BROMINATED PHENOLS. First draft prepared by Mr P.D. Howe, Dr S. Dobson, and Mr H.M. Malcolm, Centre for Ecology & Hydrology, Monks Wood, United Kingdom.	<a href="http://whqlibdoc.who.int/publications/2005/9241530669_eng.pdf">http://whqlibdoc.who.int/publications/2005/9241530669_eng.pdf</a>
USEPA Integrated Risk Information System (IRIS)	mice and rats	two 90 day gavage studies (1 in rats and 1 in mice)	Liver toxicity in female mice, as defined by an increase in liver weight and liver lesions was selected as the critical effect for deriving the chronic RfD	Toxicological review of bromobenzene (EPA/635/R-07/002) June 2007. NOTE, DRAFT REPORT NOT FOR CITATION OR QUOTATION.	<a href="http://cfpub.epa.gov/ncea/cfm/iris/recordisplay.cfm?deid=173309">http://cfpub.epa.gov/ncea/cfm/iris/recordisplay.cfm?deid=173309</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	rats & mice	rats and mice receiving bromobenzene by gavage 5 days/week for 13 weeks	liver lesions in male and female	Provisional Peer Reviewed Toxicity Values for Bromobenzene (CASRN 108-86-1). Derivation of a Chronic Oral RfD	NA
PRG region 9	unknown		unknown	USEPA Region 9. Preliminary Remediation Goals, Screening Levels for Contaminants. Accessed 18th May 2009.	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>
The Risk Assessment Information System	rat and mouse	unknown	microscopic liver lesions	Risk Assessment Information System (RAIS). Accessed 18th May 2009.	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem">http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem</a>
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	unknown		unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 20th May 2009.	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html</a>

## TDI inhal

Organisation	Study type	Description	Response	Reference	Web link
Health and Safety Executive (HSE)		retention index of VOCs		MDHS 96 volatile organic compounds in air, March 2000	<a href="http://www.hse.gov.uk/pubns/mdhs/pdfs/mdhs96.pdf">http://www.hse.gov.uk/pubns/mdhs/pdfs/mdhs96.pdf</a>
USEPA Integrated Risk Information System (IRIS)	rats and mice	two 13-week studies, one in rats and one in mice.	increased occurrence of cytomegaly and increased absolute and relative liver weight in female mice was selected as potential critical effects for deriving the subchronic RfC.	Toxicological review of bromobenzene (EPA/635/R-07/002) June 2007. NOTE, DRAFT REPORT NOT FOR CITATION OR QUOTATION.	<a href="http://cfpub.epa.gov/ncea/cfm/iris/recordisplay.cfm?deid=173309">http://cfpub.epa.gov/ncea/cfm/iris/recordisplay.cfm?deid=173309</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	mice	mice exposed tp 0, 30, 100 or 300 ppm bromobenzene 6hours/day, 5 days/week for 13 weeks.	mild centrilobular hepatocellular hypertrophy in male mice	Provisional Peer Reviewed Toxicity Values for Bromobenzene (CASRN 108-86-1). Derivation of a Chronic Inhalation RfC	NA
PRG region 9	unknown		unknown	USEPA Region 9. Preliminary Remediation Goals, Screening Levels for Contaminants. Accessed 18th May 2009.	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>
The Risk Assessment Information System	mouse	unknown	microscopic liver lesions	Risk Assessment Information System (RAIS). Accessed 18th May 2009.	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem">http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem</a>
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	unknown		unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 20th May 2009.	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html</a>

<b>Bromobenzene</b>	CAS 108-86-1	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	David Gallagher (ERM)	Final review:	Panel/SF
		Date	19/05/2009	Date	20/05/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, background exposure assumed negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 840µg/L based on a 70kg adult consuming 2L/day.
	0	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> No data, likely to be negligible
	0	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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<b>Bromodichloromethane</b>	<b>CAS Number:</b> 75-27-4	<b>Assessor A:</b> J Brown - DTS Raeburn	<b>Assessor B:</b> S Cole, URS	<b>Final review:</b> Panel/SF
		<b>Date:</b> 21/05/2009	<b>Date:</b> 10/08/2009	<b>Date:</b> 08/09/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	NR	Group 2B - probably carcinogenic to humans. No inhalation data available. IDoral applied to oral, dermal and inhalation exposure.
Apply IDoral to exposure routes?	Yes	Yes	Yes		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

<b>TDI oral</b>	<b>Recommended TDloral</b>	<b>Units</b>	<b>Justification</b>
	3	ug.kg(BW) <sup>-1</sup> .day <sup>-1</sup>	More conservative and more recently derived RfD from USEPA Health Advisors preferred to older ATSDR and IRIS health criteria.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Drinking Water Inspectorate (DWI)	<a href="http://www.dwi.gov.uk/">http://www.dwi.gov.uk/</a>		30/03/2009	DWS	100	µg/l	2.86						
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Dec-89	15/05/2009	Chronic MRL	0.018	mg/kg/day	18		LOAEL	25	mg/kg/day	1000	10 for: extrapolation from animals to humans, special variation and use of a LOAEL. LOAEL also adjusted for intermittent exposure.
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	15-11-2005	30/03/2009	Longer-term health advisory (HA)	2	mg/L	60 (assuming 70 kg adult that drinks 2 L water per day)		BMDL10	18	mg/kg-bw/day	300	Uncertainty factor based on NAS/OW guidelines. This value includes a factor of 10 to protect sensitive human populations and a factor of 10 for extrapolation from animals to humans, and a factor of 3 to account for uncertainty regarding possible reproductive effects of bromodichloromethane in humans. HA quoted in L/day in document.
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	15-11-2005	30/03/2009	RfD	0.003	mg/kg-day	3		BMDL10	0.8	mg/kg-bw/day	300	Uncertainty factor based on NAS/OW guidelines. This value includes a factor of 10 to protect sensitive human populations and a factor of 10 for extrapolation from animals to humans, and a factor of 3 to account for uncertainty regarding possible reproductive effects of bromodichloromethane in humans
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	Mar-91	18/05/2009	RfD	0.02	mg/kg/day	20	medium	LOAEL	17.9	mg/kg/day	1000	10 for: extrapolation from animals to humans, special variation and use of a LOAEL. LOAEL also adjusted for treatment schedule.
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	May-09	18/05/2009						NOAEL	20.6	mg/kg/day		

<b>TDI inhal</b>	<b>Recommended TDlinhal</b>	<b>Units</b>	<b>Justification</b>
	n/a		No information available.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
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## Bromodichloromethane

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Drinking Water Inspectorate (DWI)		This is a drinking water standard for the sum of four trihalomethanes ( chloroform, bromoform, dibromochloromethane and bromodichloromethane) and it is not possible to distinguish the proportion which might reflect BDCM contribution		The Water Supply (Water Quality) (England and Wales) Regulations 2000 SI No.3184	<a href="http://www.dwi.gov.uk/regs/si3184/3184.htm#sch1p8">http://www.dwi.gov.uk/regs/si3184/3184.htm#sch1p8</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	104wk mouse study		Renal	ATSDR, Toxicological Profile for Bromodichloromethane, 1989	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp129.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp129.pdf</a>
USEPA Health Advisors	Developmental study where drinking water administered to pregnant female rats		reduced maternal body weight gain	CCC (2000d)	<a href="http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf">http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf</a>
USEPA Health Advisors	24 month dietary study in rats		fatty degeneration in the liver of male rats	Aida et al. (1992b)	<a href="http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf">http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf</a>
USEPA Integrated Risk Information System (IRIS)	102 week mouse study	chronic mouse gavage bioassay	renal cytomegaly (kidney)	IRIS online database	<a href="http://www.epa.gov/ncea/iris/subst/0213.htm">http://www.epa.gov/ncea/iris/subst/0213.htm</a>
Toxicology Data Network (Toxnet)	30 day rat study			Aida Y, Takada K, Uchida O, Yasuhara K, Kurokawa Y, Tobe M., Toxicities of microencapsulated tribromomethane, dibromochloromethane and bromodichloromethane administered in the diet to Wistar rats for one month. Journal of Toxicological Sciences, August 1992.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~92koTn:2">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~92koTn:2</a>
TDI inhal					
Organisation	Study type	Description	Response	Reference	Web link

Bromodichloromethane		CAS Number:	75-27-4	Assessor A:	J Brown - DTS Raeburn	Assessor B:	S Cole, URS	Final review:	Panel/SF	
		Date	21/05/2009	Date	10/08/2009	Date	08/09/2009			
ID oral				Recommended IDoral	Units	Justification				
				0.3	ug.kg-1.d-1	As recommended by CLEA SR2 guidance, available BMDL10 used (3000 ug/kg/d as derived by USEPA Health Advisors from NTP study on mice) and divided by an uncertainty factor of 10,000 to give an IDoral of 0.3 ug/kg/d. This value is also very similar to the dose giving a 10-5 risk using the USEPA Health Advisors derived oral slope factor.				
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	1999	11/08/2009	Group 2B possibly carcinogenic (evidence in animals not humans)						
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2005	30/03/2009	Yes	Strong evidence of carcinogenicity in rats and mice supported by epidemiological studies showing apparent association between trihalomethanes and colorectal cancer in humans	Drinking water standard	60 (equivalent to 1.72 ug/kg/d assuming 70 kg adult that drinks 2 L water per day)	ug/L		Based on unit risks estimated using linearised multistage method on rat carcinogenicity study. The estimated range of concentrations corresponding to an upper-bound excess lifetime cancer risk of 10-5 was 25-77 µg/litre for the critical tumour types (i.e., intestinal adenomatous polyps and adenocarcinomas; renal tubular cell adenomas and adenocarcinomas) in rats and 21 µg/litre for the critical tumour types (i.e., renal adenomas and adenocarcinomas [combined]) in male mice. Previous drinking water standard of 60 ug.L-1 was kept because it lies within the concentration range for 10-5 risk from rat study and because of technical challenge of maintaining concentration of BDCM below 50 ug/L without compromising effectiveness of disinfection of water supplies.
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	May 2006	30/03/2009	Yes		Drinking water standard	16 (equivalent to 0.46 ug/kg/d assuming 70 kg adult that drinks 2 L water per day)	ug/L		Based on unit risks from incidence adenomatous polyps and carcinomas of the large intestine in rats from NTP 1987 study but resulting in a range in drinking water concentrations leading to lifetime cancer risk of 10-5 = 15.8 to 48.5 ug/L. Health Canada adopted 16 ug/L as the health criteria.
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	15/11/2005	30/03/2009	Likely human carcinogen	1) observations of tumors in animals treated by oral pathways; 2) lack of epidemiological data specific to bromodichloromethane and equivocal data for drinking water drinking water exposures that cannot reliably be attributed to bromodichloromethane among multiple other disinfection byproducts; 3) positive results for a majority of the available genotoxicity and mutagenicity tests; and 4) metabolism and mode of action that are reasonably expected to be comparable across species.	Oralslope factor	0.035 (equivalent to 0.29 ug/kg/d for lifetime cancer risk of 10-5)	(mg/kg/day) <sup>-1</sup>		Linearized multistage method used as for IRIS oral slope factor but with additional animal to human conversion factor of body weight (scaled to power).
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	15/11/2005	09/09/2009	as above	as above	LED <sub>10</sub> (the lower 95% confidence limit on a dose associated with 10% extra risk i.e. Equivalent to a BMDL <sub>10</sub> )	3000	ug/kg/d		Calculated for renal tumours in mice and assuming a linear mode of action for the carcinogenicity of bromodichloromethane

## Bromodichloromethane

ID oral					
Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)					<a href="http://www.inchem.org/documents/iarc/vol71/067-bromodicmet.html">http://www.inchem.org/documents/iarc/vol71/067-bromodicmet.html</a>
WHO Guidelines for drinking water Quality	Carcinogenesis bioassay in F344/N rats and B6C3F1 mice. Gavage with corn oil containing bromodichloromethane.	BDCM in corn oil, when administered to rats by gavage for 102 weeks at doses ranging from 50 to 100 mg/kg of body weight per day, resulted in increased incidences of renal tubular cell adenomas and adenocarcinomas affecting both sexes and a markedly increased incidence of large intestinal tumours (combined adenomas and carcinomas) in both sexes. In mice, BDCM in corn oil, administered by gavage for 102 weeks at dose levels of 0, 25, or 50 mg/kg of body weight per day or 0, 75, or 150 mg/kg of body weight per day in males and females, respectively, caused renal cytomegaly and hepatic fatty metamorphosis, increased incidences of renal tubular adenomas and carcinomas in males, and an increased incidence of combined hepatocellular adenomas and carcinomas in females.	The tumours of the large intestine (combined adenomatous polyps and carcinomas) in rats were chosen for cancer risk assessment, as they occurred with the highest frequency and affected both sexes in the study, and because of the apparent epidemiological association of this group of compounds (THMs) with colorectal cancer in humans. Furthermore, these tumours appear most likely to be associated with a mutagenic mechanism, as they were not associated with underlying cytotoxicity or other non-epigenetic mechanism. The combined large intestinal tumours had high unit risk value, equal to or higher than the unit risks for the other tumour types in rats (kidney and liver) identified in carcinogenicity studies with this compound. A cancer risk assessment was also conducted in mice, although tumours (combined renal adenomas and adenocarcinomas) were observed only in males.	NTP, 1987	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/THM200605.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/THM200605.pdf</a>
Health Canada Toxicological Values	Carcinogenesis bioassay in F344/N rats and B6C3F1 mice. Gavage with corn oil containing bromodichloromethane.	Multistage model used on NTP bioassay data described for WHO above. An allometric scaling factor was applied to the final unit risks, assuming a rat weighs 0.35 kg, a mouse weighs 0.03 kg, and a human weighs 70 kg.	in F344/N rats (i.e., intestinal adenomatous polyps and adenocarcinomas; renal tubular cell adenomas and adenocarcinomas) and in male B6C3F1 mice (renal adenomas and adenocarcinomas)	NTP, 1987	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/trihalomethanes/exposure-exposition-eng.php#a2">http://www.hc-sc.gc.ca/ewh-semt/pubs/water-eau/trihalomethanes/exposure-exposition-eng.php#a2</a>
USEPA Health Advisors	Carcinogenesis bioassay in F344/N rats and B6C3F1 mice. Gavage with corn oil containing bromodichloromethane.	As study referred to for WHO Drinking Water Standards above	Renal tumours in rats and male mice	NTP, 1987	<a href="http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf">http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf</a>
USEPA Health Advisors	as above	as above	as above	as above	as above

Bromodichloromethane		CAS Number:	75-27-4		Assessor A:	J Brown - DTS Raeburn		Assessor B:	S Cole, URS		Final review:	Panel/SF	
					Date	21/05/2009		Date	10/08/2009		Date	08/09/2009	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	Mar-93	18/05/2009	B2; probable human carcinogen	Based on inadequate human data and sufficient evidence of carcinogenicity in two animal species (mice and rats) as shown by increased incidence of kidney tumours and tumours of the large intestine in male and female rats, kidney tumours in male mice, and liver tumours in female mice	Oral slope factor	0.062 (equivalent to 0.16 ug/kg/d for lifetime cancer risk of 10 <sup>-5</sup> )	(mg/kg/day) <sup>-1</sup>	Adequate numbers of animals were used for a lifetime bioassay with two animal species. Bromodichloromethane was administered at two dose levels. Tumours of multiple tissue types were observed in a dose-related manner. Slope factors derived from tumour incidences of kidney and large intestine are similar and within one order of magnitude in differences.	Linearized multistage method used to derive cancer slope factors from 4.9e-3 to 6.2e-2 per mg/kg/d. Most conservative (6.2e-2) adopted by IRIS as the oral slope factor.			
ID inhal					Recommended IDinhal	Units	Justification						
					n/a		No information available.						
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis			

Bromodichloromethane					
Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	Carcinogenesis bioassay in F344/N rats and B6C3F1 mice. Gavage with corn oil containing bromodichloromethane.	As study referred to for WHO Drinking Water Standards above	Kidney (tubular cell adenoma and tubular cell adenocarcinoma)	NTP, 1987	<a href="http://www.epa.gov/ncea/iris/subst/0213.htm">http://www.epa.gov/ncea/iris/subst/0213.htm</a>
ID inhal					

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Drinking Water Inspectorate		drinking water			Detections of total of 4 trihalomethanes (at tap) ranged from 0 to 103.5µg/l across the 26 UK water companies in 2007. Data was not provided on any kind of average value. A total of 12,220 samples were tested with 12 failures of AC of 100µg/l		<a href="http://www.dwi.gov.uk">www.dwi.gov.uk</a>
Committee on Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)		drinking water	<50	ug/day	These compounds arise in drinking water largely as a result of disinfection, although they may also occur individually as the result of contamination. In public water supplies in England and Wales, the total concentration of the four trihalomethanes rarely exceeds 100 micrograms per litre (100 µg/l). Thus for a 60 kg individual, daily ingestion of each trihalomethane, would normally be considerably lower than 3 micrograms per kilogram body weight (3µg/kg bw).	1994 joint COC/COM/COT report	
Committee on Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)			20-200	ug/day	Level in water between 10 and 100ug/l adjusted for 2l consumption	COC, CC/07/11 - Epidemiological Studies of Chlorinated Drinking Water and Cancer, 2007	<a href="http://www.advisorybodies.doh.gov.uk/coc/index.htm">www.advisorybodies.doh.gov.uk/coc/index.htm</a>
IPCS Concise International Chemical Assessment Documents (CICADs)		drinking water	50	ug/day	Occurrence data suggest, on average, an exposure in chlorinated drinking-water to total THMs of about 35-50 µg/litre, with chloroform and BDCM being the first and second most dominant species.	UNITED NATIONS ENVIRONMENT PROGRAMME INTERNATIONAL LABOUR ORGANISATION WORLD HEALTH ORGANIZATION INTERNATIONAL PROGRAMME ON CHEMICAL SAFETY Environmental Health Criteria 216 DISINFECTANTS AND DISINFECTANT BY-PRODUCTS	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
WHO Guidelines for Drinking Water Quality		drinking water			In 1995, 3.6% of [drinking water] samples in the United Kingdom contained total trihalomethanes at concentrations above the national standard of 100 µg/l. In the Wallonia region of Belgium, the frequency of concentrations exceeding the national standard was 3.5% (41 in 1171 samples) in 1993 and 9.8% (212 in 2169 samples) in 1995. In Italy, the standard for organohalogenated compounds is 30 µg/l, but an estimated 5% of the population is supplied with water to which a waiver allowing concentrations of up to 50 µg/l is applied (91).		<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">www.who.int/water_sanitation_health/dwg/guidelines/en</a>

<b>Bromodichloromethane</b>	CAS 75-27-4	Assessor A: J Brown - DTS Raeburn	Assessor B: D Dyson, URS	Final review: Panel/SF
		Date: 21/05/2009	Date: 25/03/2009	Date: 09/09/2009

US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels		drinking water	30	ug/day	Surveys of BDCM levels in chlorinated public drinking water systems across the United States have revealed that BDCM is present in most systems at concentrations averaging around 1 to 20 µg/L, but ranging up to 125 µg/L in some cases (Coleman et al. 1975; EPA 1979; Furlong and D'itri 1986; Symons et al. 1975). The estimated exposure of the general human population to BDCM from drinking water, assuming a median BDCM concentration of 0.014 mg/L and a water intake for an adult of 2.18 L/day, would be 0.03 mg/day (EPA 1980a). Low levels of exposure might also occur by inhalation of BDCM volatilized from chlorinated water (e.g., while showering, cooking, or swimming), or by dermal contact with such water. Based on a chemical structure analogy to chloroform, an estimated dermal exposure to BDCM in a child swimming two hours/day in a saline pool would typically be 0.003 mg/day, with a maximum of 0.04 mg/day (Beech 1980). Higher exposure levels might occur through ingestion of water contaminated with BDCM near a waste site, but available data suggest that this is not a common occurrence.		
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	Dec-89	drinking water	40	ug/day	Max mean in water of 20ug/l. Adjusted for 2l consumption	ATSDR, Toxological Profile for Bromodichloromethane, 1989	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
USEPA Health Advisories		drinking water	16	ug/day	Mean of finished concs of 8.2µg/l (surface water) and 7.9µg/l (groundwater) for large-scale US supplies >100,000 persons (Disinfectants and Disinfection By products (D/DBPs) ICR Data, U.S. EPA (2001a)). Converted assuming 2L/day consumed.	see page IV - 1	<a href="http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf">http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf</a>
USEPA Health Advisories	Nov-05	drinking water	40	ug/day	converted from published mean of 20ug/l for surface water, assuming 2L/day consumed	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
Toxicological Data Network (TOXNET)	1990	drinking water	48	ug/day	converted from 24ug/l assuming 2L/day consumed	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~92koTn:2">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~92koTn:2</a>	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
Other							

MDI	Recommended MDI <sub>inhal</sub>		Units	Justification: Most conservative value from most recent study (USEPA, 2005). Published mean. Note: MDI not required as assumed to be non threshold compound
	15	ug day <sup>-1</sup>		

Organisation	Date	Media	Value	Units	Description	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	Dec-89	air			1.1ppt (mean value)	ATSDR, Toxological Profile for Bromodichloromethane, 1989	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
USEPA Health Advisories	Nov-05	outdoor air	13.4	ug/day	converted from published mean of 0.67ug/m3	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
USEPA Health Advisories	Nov-05	indoor air	15	ug/day	converted from published mean of 0.75ug/m3	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
Toxicological Data Network (TOXNET)		air	74.2	ug/day	converted from max value of 3.71 ug/m3 assuming adult breathes 20 m3/d	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~92koTn:2">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~92koTn:2</a>	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

Substance:	<b>Bromodichloromethane</b>	CAS Number:	75-27-4	Assessor A:	J Brown - DTS Raeburn	Assessor B:	D Dyson, URS	Final review:	Panel/SF
Chemical Formula:	CHBrCl2	Phase at Ambient Temperature	Liquid	Date:	21-May-09	Date:	25-Mar-09	Date:	09/09/2009

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oecd.org/scripts/hpv/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H					
							HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCK, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000					
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																																	
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	163.83	n/a	Median value chosen as central value of consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
						Average	163.83	163.83	n/a	163.829	163.829	n/a	163.829	163.829	n/a	163.83	163.83	n/a	163.83	163.83	n/a	163.83	163.83	n/a	no data	#VALUE!	n/a	163.828	163.828	n/a	163.828	163.828	n/a
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	1.62E+02	25	No consistent range - value from most recent review chosen (Montgomery 2007)		atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	KPa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	Pa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)			
						Geomean	1.60E-03	1.62E+02	20	no data	#VALUE!	no data	1.62E+02	1.72E+02	20	n/a	n/a	n/a	1.60E-03	1.62E+02	25	no data	#VALUE!	25	4.00E-01	2.22E+02	25	no data	#VALUE!	25			
							162	162	20	162	162	20	162	162	20	n/a	n/a	n/a	162	162	20	0.4	2.51E+02	no data	#VALUE!	0.4	1.97E+02	no data	#VALUE!	0.51	1.97E+02		
							192	192	20	185	185	20	192	192	20	n/a	n/a	n/a	192	192	20	0.63	1.59E+02	no data	#VALUE!	0.43	2.33E+02	no data	#VALUE!	152	152	20	
							185	185	20	185	185	20	185	185	20	n/a	n/a	n/a	185	185	20	0.48	2.09E+02	no data	#VALUE!	0.46	2.18E+02	no data	#VALUE!	185	185	20	
																n/a	n/a	n/a															
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	3.00E+03	30	No consistent range - value from most recent review chosen (Lide 2008)		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
						Geomean	4.70E+03	4.70E+03	22	3.00E+00	3000	30	2.97E+03	2.97E+03	30	No data	#VALUE!	no data	2.97E+03	3.00E+03	30	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	
Chemical Boiling Point (ambient pressure)	K	n/a	3.63E+02	n/a	Median value chosen as central value of consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	3.63E+02	n/a	n/a	3.63E+02	n/a	n/a	3.63E+02	n/a	n/a	3.62E+02	n/a	n/a	3.63E+02	n/a	n/a	#VALUE!	n/a	3.63E+02	n/a	3.63E+02	n/a	n/a	#VALUE!	n/a	363	363.00	n/a
							90	363.15	n/a	90	363.15	n/a	90	363.15	n/a	88.4	361.55	n/a	90.1	363.25	n/a	no data	#VALUE!	n/a	363	363.00	n/a	no data	#VALUE!	n/a	n/a	n/a	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Chemical Melting Point (ambient pressure)	K	n/a	2.16E+02	n/a	Median value chosen as central value of consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	2.16E+02	n/a	n/a	2.16E+02	n/a	n/a	2.16E+02	n/a	n/a	#VALUE!	n/a	n/a	2.16E+02	n/a	n/a	#VALUE!	n/a	216	216.00	n/a	216	216.00	n/a	no data	#VALUE!	n/a	
							-57.1	216.05	n/a	-57	216.15	n/a	-57	216.15	n/a	no data	#VALUE!	n/a	-57.1	216.05	n/a	no data	#VALUE!	n/a	216	216.00	n/a	no data	#VALUE!	n/a	n/a	n/a	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Log Octanol - Water Coefficient	Dimensionless	n/a	2.02E+00	n/a	Median value chosen as central value of consistent range		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
						Average	2.1	2.10	n/a	no data	Insert Values	n/a	1.88	1.88	n/a	no data	Insert Values	n/a	1.88	1.88	n/a	no data	Insert Values	n/a	no data	Insert Values	n/a	no data	Insert Values	n/a	no data	Insert Values	n/a
							2.1	2.10	n/a	no data	no data	n/a	2.1	2.10	n/a	no data	no data	n/a	2.1	2.10	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Molar Volume (Le Bas method)	cm3 mol <sup>-1</sup>	n/a	9.47E+01	n/a	single literature value		cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)
						Average	n/a	n/a	n/a	n/a	n/a	n/a	94.7	94.70	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	32357.73477	3.24E+04	Normal Chemical Boiling Point	Calculated value chosen		KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)
						Average	n/a	n/a	n/a	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!
							n/a	n/a	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Chemical Critical Point temperature (ambient pressure)	K	585.8543164	585.85	n/a	Calculated value chosen		K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	n/a	n/a	n/a	no data	Insert Values	n/a	no data	no data	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
							n/a	n/a	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Critical Pressure	atm	57.36143692	57.36	n/a	Calculated value chosen		Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)
						Average	n/a	n/a	n/a	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!	no data	#VALUE!
							n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	3.19E-02	10	Estimated from parameters above using Clapyron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	3789	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale

<b>Bromoform</b>	<b>CAS Number:</b> 75-25-2	<b>Assessor A:</b> J Brown - DTS Raeburn	<b>Assessor B:</b> A Fellows - Ecologia	<b>Final review:</b> Panel/SF
		<b>Date:</b> 03/04/2009	<b>Date:</b> 06/04/2009	<b>Date:</b> 28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen - TDloral applied to oral and dermal routes.  Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen. Insufficient data on inhalation toxicity to derive TDlinhal. TDloral applied to inhalation routes.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	20	ug.kg-1.d-1	Most conservative value with good agreement between sources (WHO rounded up value, RIVM and USEPA IRIS)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	2001	09/04/2009	no data	no data	no data	no data	no data	no data	25	mg/kg-day	no data	no data
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	2000	05/04/2009	TDI	25	µg/kg	25	no data	NOAEL	25	mg/kg bw/day	1000	10 each for inter- and intraspecies variation and 10 for the short duration of the study and possible carcinogenicity
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2008	08/04/2009	TDI	25	µg/kg bw 5 days/week	17.9	no data	NOAEL	25	mg/kg bw/day	1000	100 for intra and interspecies variation and 10 for possible carcinogenicity and short duration of the study
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2005	09/04/2009	TDI	20	µg/kg bw/day	20	no data	NOAEL	20	mg/kg bw/day	1000	factor of 10 for use of a subchronic assay, 10 for extrapolation of animal data to humans, factor 10 for the protection of sensitive human sub population.
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Aug-05	06/04/2009	MRL acute	0.7	mg/kg/day	700	no data	NOAEL	72	mg/kg/day	100	10 for animal to human extrapolation and 10 for human variability
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Aug-05	06/04/2009	MRL intermediate	0.2	mg/kg/day	200	no data	NOAEL	18	mg/kg/day	100	10 for animal to human extrapolation and 10 for human variability
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/dinking">http://www.epa.gov/waterscience/criteria/dinking</a>	2005	09/04/2009	RfD	0.03	mg/kg-day	30	no data	NOAEL	25	mg/kg-day	100	Composite uncertainty factor based on NAS/OW guidelines; includes a factor of 10 for interspecies variation, a factor of 10 for protection of sensitive human populations
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1989	08/04/2009	RfD	0.02	mg/kg/day	20	Medium	NOAEL	25	mg/kg-day	1000	Factors of 10 were employed for use of a subchronic assay, for extrapolation from animal data, and for protection of sensitive human subpopulation.
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	2005	03/08/2009	subchronic RfD	0.03	mg/kg/day	30	no data	BMDL	2.6	mg/kg/day	100	10 for animal to human extrapolation and 10 for human variability
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	1997	09/04/2009	Oral	0.2	mg/kg/day	200	no data	no data	no data	no data	no data	no data

TDI inhal	Recommended TDlinhal	Units	Justification
		ug.kg-1.d-1	Insufficient data on inhalation pathway to derive TDI inhal. Route to route extrapolation from oral TDI applied.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2005	09/04/2009	TCA	100	µg/m³	28.57	no data	no data	no data	no data	no data	Already applied

Bromoform		CAS Number:	75-25-2	Assessor A:	J Brown - DTS Raeburn	Assessor B:	A Fellows - Ecologia	Final review:	Panel/SF			
				Date	03/04/2009	Date	06/04/2009	Date	28/08/2009			
<b>ID oral</b>				<b>Recommended IDoral</b>	n/a		<b>Units</b>	<b>Justification</b>				
								Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen				
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating		Basis	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/01/1991	09/04/2009	B2 - probable human carcinogen	Based on inadequate human data and sufficient evidence of carcinogenicity in animals	oral slope factor	0.0079	mg/kg/day				Extrapolation Method — Linearized multistage procedure, extra risk
<b>ID inhal</b>				<b>Recommended IDinhal</b>	n/a		<b>Units</b>	<b>Justification</b>				
								Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen				
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating		Basis	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/01/1991	09/04/2009	B2 - probable human carcinogen	Based on inadequate human data and sufficient evidence of carcinogenicity in animals	oral slope factor	0.000011	mg/kg/day				Extrapolation Method — Linearized multistage procedure, extra risk

## Bromoform

## TDI oral

Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	Animal	unknown	liver toxicity	Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment, TOX/2001/16 - A Sahu Study on Chlorination Disinfection By-Products and Birth Outcomes in 3 Water Areas in England, 2001 (For members use only)	<a href="http://cot.food.gov.uk/pdfs/tox200116.pdf">http://cot.food.gov.uk/pdfs/tox200116.pdf</a>
International Programme on Chemical Safety (IPCS)	13 weeks after dosing by corn oil gavage	Rats	Absence of Liver Lesions	IPCS, Environmental Health Criteria 216 - Environmental Health Criteria for Disinfectants and Disinfectant By-Products, 2000	<a href="http://www.inchem.org/documents/ehc/ehc/ehc216.htm">http://www.inchem.org/documents/ehc/ehc/ehc216.htm</a>
WHO Guidelines for drinking water Quality	90 days	Rats	absence of histopathological lesions in the liver	WHO, Guidelines for Drinking Water Quality, 2008	<a href="http://www.who.int/water_sanitation_health/dwg/2edvol1c.pdf">http://www.who.int/water_sanitation_health/dwg/2edvol1c.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	7 days/week for 13 weeks	Rats	Hepatic Lesions	Janssen et al. Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998.	<a href="http://www.rivm.nl/bibliotheek/rapporten/601501027.html">http://www.rivm.nl/bibliotheek/rapporten/601501027.html</a> <a href="http://rivm.openrepository.com/rivm/bitstream/10029/10310/1/711701004.pdf">http://rivm.openrepository.com/rivm/bitstream/10029/10310/1/711701004.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	short duration - Corn oil 5 days/week for 13 weeks	rats	Minimal to moderate liver and kidney histological alterations were observed	ATSDR, Toxicological Profile for Bromoform and Dibromochloromethane, 2005	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp130.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp130.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Intermediate duration - Corn oil 5 days/week for 13 weeks	Rats	hepatocellular vacuolization	ATSDR, Toxicological Profile for Bromoform and Dibromochloromethane, 2005	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp130.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp130.pdf</a>
USEPA Health Advisors	5 days/week for 13 weeks (subchronic)	Rats, gavage in corn oil	histopathological changes (vacuolization) in the liver.	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf">http://www.epa.gov/waterscience/criteria/drinking/brthm-200605(508).pdf</a>
USEPA Integrated Risk Information System (IRIS)	5 days/week for 13 weeks (subchronic)	Rat, Gavage Bioassay	Hepatic Lesions	IRIS online database. Last updated in 1989	<a href="http://www.epa.gov/ncea/iris/subst/0214.htm">http://www.epa.gov/ncea/iris/subst/0214.htm</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	13 week study	male rats	hepatocellular vacuolization	Superfund Health Risk Technical Support Centre, Provisional Peer Reviewed Toxicity Values for Bromoform (2005)	n/a
Toxicology Data Network (Toxnet)	13 week, subchronic	Rats, Gavage Study	Liver Lesions	Bromoform - Anonymous (1997)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~cnjals:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~cnjals:1</a>

## TDI inhal

Organisation	Study type	Description	Response	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Animal Study	only accounts for systemic effects of inhalation and is derived from oral TDI		Janssen et al. Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998.	<a href="http://rivm.openrepository.com/rivm/bitstream/10029/10310/1/711701004.pdf">http://rivm.openrepository.com/rivm/bitstream/10029/10310/1/711701004.pdf</a>

## Bromoform

ID oral

Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	animal (rat) carcinogenesis rates. Test Species: F344/N rat, female	by gavage in corn oil	Tumor Type: Neoplastic lesions in the large intestine	IRIS online database. Last updated in 1993	<a href="http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nbr=0214#carc">http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nbr=0214#carc</a>

ID inhal

Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	animal (rat) carcinogenesis rates. Test Species: F344/N rat, female	by gavage in corn oil	Tumor Type: Neoplastic lesions in the large intestine	IRIS online database. Last updated in 1993	<a href="http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nbr=0214#carc">http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nbr=0214#carc</a>

Bromoform	CAS 75-25-2	Assessor A:	J Brown - DTS Raeburn	Assessor B:	A Fellows - Ecologia	Final review:	Panel/SF
		Date	05/04/2009	Date	06/04/2009	Date	28/08/2009

MDI	Recommended MDI <sub>oral</sub>	Units	Justification: ATSDR exposure value from drinking water, converted assuming an adult bodyweight (x 70kg). Exposure still fairly conservative in consideration of the COT report. COT data is inappropriate as document is for 'members use only'.
	42	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	2001	drinking water	70	ug day-1	uk specific exposure from drinking water "in the order of 1ug/kg/day"	Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment, TOX/2001/16 - A Sahu Study on Chlorination Disinfection By-Products and Birth Outcomes in 3 Water Areas in England, 2001 (For members use only)	<a href="http://www.cot.food.gov.uk">www.cot.food.gov.uk</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	2005	drinking water	42	ug day-1	converted from 0.6ug/kg/day	ATSDR, Toxicological Profile for Bromoform and Dibromochloromethane, 2005	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
USEPA Health Advisories	2005	drinking water	2.4	ug day-1	Median surface supplies exposure	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
			Recommended MDI <sub>inhal</sub>	Units	Justification: RIVM report. Value is also most conservative, converted assuming an adult bodyweight (x 70kg). In close agreement with USEPA value for outdoor air		
			70	ug day-1			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	2005	air	70	ug day-1	converted from background exposure of <1ug/kg/day.	Janssen et al. 1998 based on US EPA IRIS (1995). Maximum Permissible Risk Levels for Human Intake of Soil Contaminants: Fourth Series of Compounds. RIVM Report No. 711701004. March 1998.	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	2005	air	0.7	ug day-1	converted from 0.01ug/day	ATSDR, Toxicological Profile for Bromoform and Dibromochloromethane, 2005	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
USEPA Health Advisories	2005	outdoor air in suburban/urban USA	64	ug day-1	converted from max concentration of 3.2ug/m3	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
USEPA Health Advisories	2005	indoor air	7	ug day-1	converted from max concentration of 0.35ug/m3	EPA Office of Water, Drinking Water Criteria Document for Brominated Trihalomethanes, 2005	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>



Butyl benzyl phthalate	CAS Number: 85-68-7	Assessor A: N Struggles, AECOM	Assessor B: Atkins	Final review: Panel/SF
		Date: 01/06/2009	Date: 17/06/2009	Date: 26/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDioral to exposure routes?	Yes	Yes	Yes	Yes	Insufficient data to assess non threshold effects - so HCV based on threshold effects. Route to route extrapolation from oral HCV
Apply IDoral to exposure routes?	No	No	No		
Apply TDInh to exposure routes?	No	No	No		
Apply IDInh to exposure routes?	No	No	No		

TDI oral	Recommended TDIORal	Units	Justification
	500	ug.kg-1.d-1	EFSA and Dutch RIVM most recent studies and report same value.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
European Food Safety Authority (EFSA)	<a href="http://www.efsa.europa.eu/en.html">http://www.efsa.europa.eu/en.html</a>	No data	01/06/2009	TDI	0.5	mg/kg bw/day	500	n/a	NOAEL	50	mg/kg bw/day	100	10 each for inter and intraspecies differences (EFSA)	Rat, oral
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://incem.org/pages/cicads.html">http://incem.org/pages/cicads.html</a>	01/01/1999	01/06/2009	TDI oral	1.3	mg.kgbw-1.d-1	1300	Medium	Benchmark Dose	132	mg.kgbw-1.d-1	100	Inter and Intra species variation	Subchronic
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/03/2001	01/06/2009	TDI oral	500	ug.kgbw-1.d-1	500	Medium	NOAEL	151	mg.kg-1.d-1	300	Inter and Intra species variation	Subchronic
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>		25/03/2009	Benchmark Dose	1.3	mg/kg bw/day	1300	Moderate to high	lower 95th confidence interval of Benchmark Dose	132	mg/kg bw/day	100	Inter and intraspecies variations (10 each) (Health Canada)	Subchronic
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/02/1993	01/06/2009	RfD	0.2	mg.kg-1.d-1	200	Medium	NOAEL	159	mg.kg-1.d-1	1000	10 for intraspecies sensitivity, 10 for interspecies variability and 10 for extrapolating from subchronic to chronic NOAEL.	Repeat dose study
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	01/10/2002	n/a	Provisional Oral Slope Factor	0.0019	mg/kg-day	n/a	n/a	n/a	n/a	n/a	n/a	n/a	Rat, oral

TDI inhal	Recommended TDInhal	Units	Justification
			Insufficient data with sufficient detail on derivation to derive a TDInhal. Use route-to-route extrapolation from oral.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://incem.org/pages/cicads.html">http://incem.org/pages/cicads.html</a>	1999	25/03/2009	none						51	mg/m3			Rat, inhalation
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	01/03/2001	01/06/2009		Due to low volatility of BBP inhalation exposure is considered not relevant									

## Butyl benzyl phthalate

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
European Food Safety Authority (EFSA)	multigenerational reproductive and developmental study	reduced anogenital distance (AGD) in F1 (1st generation) and F2 at birth (2nd generation) rats.	The EFSA Journal (2005) 241. Butylbenzylphthalate in food contact materials	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej24_1_bbp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej24_1_bbp_en2.pdf?ssbinary=true</a>
IPCS concise International Chemical Assessment Documents (CICADs)	Hammond et al. 1987 3 month dietary study of male Wistar rats	Pancreatic lesions	Concise International Chemical Assessment Document 17 1999 BUTYL BENZYL PHTHALATE	<a href="http://incchem.org/documents/cicads/cicads/cicad17.htm#SectionNumber:6.2">http://incchem.org/documents/cicads/cicads/cicad17.htm#SectionNumber:6.2</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels.	3 month study with rats effects on kidney weight and urinary pH were noticed, NOAEL of 151 mg.kg-1.d-1. NTP 1997 study marginal effects noticed on haemoglobin concentrations at 550 mg.kg-1.d-1 after 26 weeks. At higher dose levels testicular atrophy was found. NOAEL of 2800 ppm in the diet, which is 161 mg.kg-1.d-1.	Kidney; Testicular atrophy	Baars et al. 2001 'Re-evaluation of human-toxicological maximum permissible risk levels' RIVM report 711701 025.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
Health Canada Toxicological Values	Rat, oral study	A 5% increase in the incidence of pancreatic lesions in male Wistar rats.	Hammond, B.G., G.J. Levinskas, E.C. Robinson and F.R. Johansen. 1987. A review of the subchronic toxicity of butyl benzyl phthalate. Toxicol. Ind. Health 3(2): 79-98. Cited in Health Canada, 2000. Canadian Environmental Protection Act. Priority substances list assessment report: Butylbenzylphthalate	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/psl2-lsp2/butylbenzylphthalate/butylbenzylphthalate-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/psl2-lsp2/butylbenzylphthalate/butylbenzylphthalate-eng.pdf</a>
USEPA Integrated Risk Information System (IRIS)	NTP (1985) conducted a toxicity study in F344 rats in which 15 males/group were administered concentrations of either 0, 0.03, 0.09, 0.28, 0.83, or 2.5% BBP in the diet for 26 weeks	Reduction in relative brain and liver weights	USEPA IRIS	<a href="http://www.epa.gov/ncea/iris/subst/0425.htm">http://www.epa.gov/ncea/iris/subst/0425.htm</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	NTP (1997) study based on the increase in pancreatic cancer in male F334 rats through a 2 year feeding study. Slope factor derived within the PPRTV using the proposed guidelines (U.S. EPA, 1996a, 1999).	Pancreatic acinar cell adenoma and acinar cell adenoma or carcinoma	Provisional Peer Reviewed Toxicity values for Butylbenzyl Phthalate (CASRN 85-68-7) Derivation of a Carcinogenicity Assessment.	n/a
TDI inhal				
Organisation	Description	Response	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)	Subchronic inhalation study in rats - endpoints examined were limited to organ weights and histopathology.	Adverse effects on body weight gain and serum glucose.	World Health Organization International Programme on Chemical Safety, 1999. Concise International Chemical Assessment Document 17: BUTYL BENZYL PHTHALATE	<a href="http://incchem.org/documents/cicads/cicads/cicad17.htm">http://incchem.org/documents/cicads/cicads/cicad17.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			Baars et al. 2001 'Re-evaluation of human-toxicological maximum permissible risk levels' RIVM report 711701 025.	

Butyl benzyl phthalate		CAS Number:	85-68-7	Assessor A:	N Struggles, AECOM	Assessor B:	Atkins	Final review:	Panel/SF		
				Date	01/06/2009	Date	17/06/2009	Date	26/08/2009		
<b>ID oral</b>						<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>			
						None		Insufficient data			
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	No data	01/06/2009	Weight of evidence is that BBP is not a human carcinogen							
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	No data	01/06/2009	Conclude little evidence that BBP is a human carcinogen.							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	28/10/2003	01/06/2009	Possible human carcinogen Based on statistically significant increase in mononuclear cell leukaemia in female rats; the response in male rats was inconclusive and there was no such response in mice.							
<b>ID inhal</b>						<b>Recommended IDinhal</b>	<b>Units</b>	<b>Justification</b>			
						None		Insufficient data			
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	No data	01/06/2009	Weight of evidence is that BBP is not a human carcinogen							
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	No data	01/06/2009	Conclude little evidence that BBP is a human carcinogen.							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	No data	01/06/2009	Possible human carcinogen Based on statistically significant increase in mononuclear cell leukaemia in female rats; the response in male rats was inconclusive and there was no such response in mice.							

Butyl benzyl phthalate

ID oral				
Organisation	Description	Response	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)			Concise International Chemical Assessment Document 17 1999 BUTYL BENZYL PHTHALATE	<a href="http://inchem.org/documents/cicads/cicads/cicad17.htm#SectionNumber:6.2">http://inchem.org/documents/cicads/cicads/cicad17.htm#SectionNumber:6.2</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			Baars et al. 2001 'Re-evaluation of human-toxicological maximum permissible risk levels' RIVM report 711701 025.	
USEPA Integrated Risk Information System (IRIS)			USEPA IRIS	<a href="http://www.epa.gov/ncea/iris/subst/0425.htm">http://www.epa.gov/ncea/iris/subst/0425.htm</a>
ID inhal				
Organisation	Description	Response	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)			Concise International Chemical Assessment Document 17 1999 BUTYL BENZYL PHTHALATE	<a href="http://inchem.org/documents/cicads/cicads/cicad17.htm#SectionNumber:6.2">http://inchem.org/documents/cicads/cicads/cicad17.htm#SectionNumber:6.2</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			Baars et al. 2001 'Re-evaluation of human-toxicological maximum permissible risk levels' RIVM report 711701 025.	
USEPA Integrated Risk Information System (IRIS)			USEPA IRIS	<a href="http://www.epa.gov/ncea/iris/subst/0425.htm">http://www.epa.gov/ncea/iris/subst/0425.htm</a>

<b>Butyl benzyl phthalate</b>	CAS 85-68-7	Assessor A:	N Struggles, AECOM	Assessor B:	Atkins	Final review:	Panel/SF
		Date	01/06/2009	Date	17.06.2009	Date	26/08/2009

<b>MDIoral</b>	<b>Recommended MDIoral</b>	<b>Units</b>	<b>Justification:</b> Intake from water anticipated to be low (EFSA). Therefore based on mean dietary intake for UK population (EFSA).
	<b>8</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
European Food Safety Authority (EFSA)	01/05/2009	Diet	0.008; 0.02	mg/day	Mean and 97th percentile dietary intake for UK population (upper end of range) from 1993 Total Diet Study. Mean selected.	The EFSA Journal (2005) 241. Butylbenzylphthalate in food contact materials. http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej241_bbp_en2.pdf?ssbinary=true	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	01/05/2009	All routes oral	2	ug. kg bw-1.d-1	Estimated intake for adults for all oral sources (drinking water and diet) based on information provided by Health Canada. Although concentrations of BBP in air (both ambient and indoor), drinking-water, and soil have been reported, they are so low that intakes from these routes are essentially negligible. Estimates of exposure for the general population are based almost entirely upon the estimates for intake from food.	Section 7. World Health Organization International Programme on Chemical Safety, 1999. Concise International Chemical Assessment Document 17: BUTYL BENZYL PHTHALATE	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	01/05/2009	Food	2 to 6	ug. kg bw-1.d-1	Based on CICADs Total intake therefore 6 ug/kg-bw/day x 70kg = 420ug/day	Baars et al. 2001 'Re-evaluation of human-toxicological maximum permissible risk levels' RIVM report 711701 025.	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
Health Canada Toxicological Reference Values	08/05/2009	Daily exposure from dietary and drinking water sources	14.06	ug/kg bw/day	Daily exposure for 20-59 yr old adults - Sum of upper range of 14 and 0.06 ug/kg bw/day from dietary and drinking water sources, respectively.	Health Canada, 2000. Canadian Environmental Protection Act. Priority substances list assessment report: Butylbenzylphthalate	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>

<b>Butyl benzyl phthalate</b>	CAS 85-68-7	Assessor A:	N Struggles, AECOM	Assessor B:	Atkins	Final review:	Panel/SF
		Date	01/06/2009	Date	17.06.2009	Date	26/08/2009

<b>MDIinhal</b>	<b>Recommended MDlinh</b>	<b>Units</b>	<b>Justification:</b> IPCS state that uptake from air is negligible. Data selected from Spain rather than the US or Canada. 2ng/m3 selected, converted assuming an adult breathes 20m3/day x 1/1000 ug/ng. Worst case value selected based on fine aerosol fractions (<0.5um fraction), in summer.
	<b>0.04</b>	<b>ug day-1</b>	

Organisation		Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	08/05/2009	outdoor air samples	a) 6.7 b) 1.0 and 8.0ng/m3 in winter c) 0.25 and 2.0 ng/m3 in summer d) negligible	ng/m3	a) Outdoor levels for California, measured at night - 90th percentile value. b), c) Ambient air in Barcelona, Spain. Concentrations in winter and summer, associated with coarse (>7.2 µm) and fine (<0.5 µm) aerosol fractions, respectively, have been reported (Aceves & Grimalt, 1993). d) Although concentrations of BBP in air (both ambient and indoor), drinking-water, and soil have been reported, they are so low that intakes from these routes are essentially negligible.	World Health Organization International Programme on Chemical Safety, 1999. Concise International Chemical Assessment Document 17: BUTYL BENZYL PHTHALATE	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Health Canada Toxicological Reference Values	08/05/2009	ambient air daily exposure	0.001	ug/kg bw/day	Daily exposure for 20-59 yr old adults - upper end of range from ambient air source only.	Canadian Environmental Protection Act. Priority substances list assessment report: Butylbenzylphthalate	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>



Carbazole	CAS Number:	86-74-8	Assessor A: Simon Clennell-Jones (WSP)	Assessor B: Simon Tempest (ERM)	Final review: Panel/SF	
	Date	19/05/2009	Date	20/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	NR	Group 3 IARC Not classifiable as to its carcinogenicity to humans. Group B2 USEPA Probably carcinogenic to humans (little or no human data). Insufficient data with sufficient details to derive TDIs or IDs.
Apply IDoral to exposure routes?	Yes	Yes	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	Yes		

TDI oral					Recommended TDloral	Units	Justification						
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	NR	14/05/2009										
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	NR	14/05/2009										
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	NR	14/05/2009										
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/jecfa/en/">http://who.int/ipcs/food/jecfa/en/</a>	NR	18/05/2009										
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	23/07/2008	NA	RFD PPRTV	inadequate data to derive a p-RFD								

TDI inhal					Recommended TDlinhal	units	CLEA Units ug.kg-1.d-1	Justification					
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	23/07/2008	NA	RFC PPRTV	No inhalation toxicity data identified to derive a p-RFC								

ID oral					Recommended IDoral	Units	Justification						
Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Value	Units	UF	UF description
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	12/03/2009	18/05/2009										

## Carbazole

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
European Chemicals Bureau (ECB)	rat	Acute oral toxicity data (report not in English). Quotes >16000 mg/kg bw and >5000 mg/kg bw (page 20).		luclid dataset. European commission - European chemicals bureau. 19 February 2000.	<a href="http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/IUCLID/DATA_SHEETS/91995163.pdf">http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/IUCLID/DATA_SHEETS/91995163.pdf</a>
Scientific Committee on Food (SCF) pre 2002			Skin	Commission recommendation of 19/09/2003 concerning the European schedule of occupational diseases	<a href="http://ec.europa.eu/employment_social/news/2003/sep/occdis_recc_en.pdf#xml=http://158.167.146.104:7001/www/xmlread.jsp?ServerSpec=158.167.146.104:9000&amp;K2DocKey=http%3A%2F%2Fec.europa.eu%2Femployment_social%2Fnews%2F2003%2Fsep%2Foccdis_recc_en.pdf%40EUROPACORE_ece_u_x&amp;QueryText=carbazole">http://ec.europa.eu/employment_social/news/2003/sep/occdis_recc_en.pdf#xml=http://158.167.146.104:7001/www/xmlread.jsp?ServerSpec=158.167.146.104:9000&amp;K2DocKey=http%3A%2F%2Fec.europa.eu%2Femployment_social%2Fnews%2F2003%2Fsep%2Foccdis_recc_en.pdf%40EUROPACORE_ece_u_x&amp;QueryText=carbazole</a>
International Agency for Research on Cancer (IARC)	mice	In a study by oral administration, a dose-dependent increase in the incidence of liver neoplastic nodules and hepatocellular carcinomas was observed. Papillomas and carcinomas of the forestomach occurred in animals receiving the high-dose level. There is limited evidence that carbazole is carcinogenic to experimental animals.	liver and forestomach	International Agency for Research on Cancer (IARC) - Summaries & Evaluations. Carbazole. VOL.: 32 (1983) (p. 239)	<a href="http://www.inchem.org/documents/iarc/vol32/carbazole.html">http://www.inchem.org/documents/iarc/vol32/carbazole.html</a>
Joint Expert Committee on Food Additives (JECFA)				Page 94 - IARC classification of carbazole (classed as level 3 - the compound is not classifiable as to its carcinogenicity to humans).	<a href="http://whqlibdoc.who.int/publications/2004/9241530626.pdf">http://whqlibdoc.who.int/publications/2004/9241530626.pdf</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				Provisional Peer Reviewed Toxicity Values for Carbazole (CASRN 86-74-8).	NA
TDI inhal					
Organisation	Study type	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				Provisional Peer Reviewed Toxicity Values for Carbazole (CASRN 86-74-8).	NA
ID oral					
Organisation	Study type	Description	Response	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels				Agency for toxic substances & disease registry- public health assessment. Reference to the EPA's Oral Cancer Slope Factor (mg/kg/day)-1 - quotes 0.02.	<a href="http://www.atsdr.cdc.gov/HAC/PHA/oakridge013107-TN/ceo_p4.html#t21">http://www.atsdr.cdc.gov/HAC/PHA/oakridge013107-TN/ceo_p4.html#t21</a>

Carbazole		CAS Number:	86-74-8	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	Simon Tempest (ERM)	Final review:	Panel/SF
				Date:	19/05/2009	Date:	20/05/2009	Date:	28/08/2009
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	NR	14/05/2009						
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	23/07/2008	NA		Oral slope factor could not be derived due to lack of suitable oral data in humans or animals. PPRTV included a review of HEAST database.				
PRG region 9	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>	Oct-04	18/05/2009	unknown	Slope Factor Sourced from HEAST	oral slope factor	0.02	(mg/kg/bw.day)-1	unknown
The Risk Assessment Information System	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem">http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem</a>	1986	18/05/2009	liver tumour	Slope Factor Sourced from HEAST	oral slope factor	0.02	(mg/kg/bw.day)-1	unknown
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html</a>	26/03/2009	19/05/2009	unknown	Slope Factor Sourced from HEAST	oral slope factor	0.02	(mg/kg/bw.day)-1	unknown

ID inhal					Recommended IDoral	Units	Justification						
						µg/kg/day	Insufficient data with sufficient detail to derive ID						
Organisation		Last Updated		Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating				Basis
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	23/07/2008	NA										
PRG region 9	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>	Oct-04	18/05/2009			inhalation slope factor (extrapolated oral)	0.02	(mg/kg/bw.day)-1	unknown				

## Carbazole

USEPA Integrated Risk Information System (IRIS)		From website (need to purchase report at \$15) - Carbazole has been evaluated as a carcinogen. The human carcinogen potency factor (q1*) for carbazole is .028/(mg/kg/day)-1 for oral exposure.		Health and Environmental Effects Profile for Carbazole. Environmental Protection Agency, Cincinnati, OH. Environmental Criteria and Assessment Office (only available to purchase)	<a href="http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=34385">http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=34385</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				Provisional Peer Reviewed Toxicity Values for Carbazole (CASRN 86-74-8).	NA
PRG region 9	unknown		unknown	USEPA Region 9. Preliminary Remediation Goals, Screening Levels for Contaminants. Accessed 18th May 2009.	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>
The Risk Assessment Information System	mouse	unknown	Liver Tumours	Risk Assessment Information System (RAIS). Accessed 18th May 2009.	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem">http://rais.ornl.gov/cgi-bin/tox/TOX_select?select=chem</a>
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	unknown		unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 19th May 2009.	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppls.html</a>

ID inhal					
Organisation	Study type	Description	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)				Provisional Peer Reviewed Toxicity Values for Carbazole (CASRN 86-74-8).	NA
PRG region 9	unknown		unknown	USEPA Region 9. Preliminary Remediation Goals, Screening Levels for Contaminants. Accessed 18th May 2009.	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtable.pdf</a>

Carbazole	CAS 86-74-8	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	Simon Tempest (ERM)	Final review:	Panel/SF
		Date	19/05/2009	Date	20/05/2009	Date	28/08/2009

MDI	Recommended MDloral	Units	Justification: No data, likely to be negligible.
	0	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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MDI	Recommended MDlinh	Units	Justification: No data, likely to be negligible.
	0	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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Substance:		Carbozole	CAS Number:		86-74-8	Assessor A:		Simon Clennell-Jones (WSP)	Assessor B:		Alan Wilson (ERM)	Final Review:		Panel/SF																	
Chemical Formula:		C <sub>12</sub> H <sub>9</sub> N	Phase at Ambient Temperature:		Solid	Date:		11.04.2009	Date:		18.05.2009	Date:		28.08.2009																	
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIJE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000			
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units
<b>Required Parameters</b>																															
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	167.206	n/a	Consistent Value		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	
						Average	Insert Values	n/a	n/a	167.206	167.206	n/a	167.206	167.206	n/a	167.206	167.206	n/a	167.21	167.21	n/a	167.21	167.21	n/a	167.2066	167.2066	n/a	167.2066	167.2066	n/a	
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	16.00	25	Single Value		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	
						Geomean	Insert Values	25	25	Insert Values	25	25	25	16	16	25	n/a	n/a	n/a	Insert Values	25	25	25	25	25	25	25	25	25	25	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	1.164	25	Median Value From Consistent Range		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	
						Geomean	Insert Values	0.0012	1.2	25	1.037	1.04E+00	25	1.67	1.67E+00	25	1.03	1.03E+00	25	0.908	9.08E-01	25									
Chemical Boiling Point (ambient pressure)	K	n/a	627.99	n/a	Median Value From Consistent Range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	
						Average	Insert Values	n/a	n/a	354.69	6.28E+02	n/a	354.69	6.28E+02	n/a	355	628.15	n/a	Insert Values	n/a	Insert Values	n/a	628.2	628.20	n/a	628.2	628.20	n/a	628.2	628.20	n/a
Chemical Melting Point (ambient pressure)	K	n/a	519.45	n/a	Consistent Value		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	
						Average	Insert Values	n/a	n/a	246.3	5.19E+02	n/a	246.3	5.19E+02	n/a	245	518.15	n/a	Insert Values	n/a	Insert Values	n/a	519.45	519.45	n/a	519.45	519.45	n/a	519.45	519.45	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	3.60	n/a	Median Value From Consistent Range		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	
						Average	Insert Values	n/a	n/a	3.72	3.72	n/a	3.29	3.29	n/a	3.01	3.01	n/a	3.5	3.50	n/a	3.72	3.72	n/a	3.59	3.59	n/a	3.84	3.84	n/a	
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	192.9	n/a	Single Value		n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
						Average	n/a	n/a	n/a	192.9	192.90	n/a	192.9	192.90	n/a	192.9	192.90	n/a	192.9	192.90	n/a	192.9	192.90	n/a	192.9	192.90	n/a	192.9	192.90	n/a	192.9
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	59950.0906	59,950	Normal Chemical Boiling Point	Calculated Value		n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>		KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>		n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
						Average	n/a	n/a	n/a	58.569	5.86E+04	Normal Boiling Point	58.569	5.86E+04	Normal Boiling Point	58.569	5.86E+04	Normal Boiling Point	58.569	5.86E+04	Normal Boiling Point	58.569	5.86E+04	Normal Boiling Point	58.569	5.86E+04	Normal Boiling Point	58.569	5.86E+04	Normal Boiling Point	
Chemical Critical Point temperature (ambient pressure)	K	898.8441	898.8	n/a	Calculated Value		n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
						Average	n/a	n/a	n/a	901.8	9.02E+02	n/a	901.8	9.02E+02	n/a	901.8	9.02E+02	n/a	901.8	9.02E+02	n/a	901.8	9.02E+02	n/a	901.8	9.02E+02	n/a	901.8	9.02E+02	n/a	
Critical Pressure	atm	32.2214	32.22	n/a	Calculated Value		n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
						Average	n/a	n/a	n/a	31.3	3.09E+01	n/a	31.3	3.09E+01	n/a	31.3	3.09E+01	n/a	31.3	3.09E+01	n/a	31.3	3.09E+01	n/a	31.3	3.09E+01	n/a	31.3	3.09E+01	n/a	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	0.00115	10	Estimated from parameters above using Clapron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	7.63576E-06	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	5.39E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	4.40E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	2.89	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Chloroethane	CAS Number: 75-00-3	Assessor A: Jane Thrasher (Jacobs)	Assessor B: Andy Singleton (ESI)	Final review: Panel/SF
		Date: 29/04/2009	Date: 30/04/2009	Date: 26/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	NR	Insufficient data with sufficient information on derivation to derive TDloral. Route to route extrapolation to oral and dermal routes from inhalation TDI used.  Carcinogenic category 3 (IARC): no strong evidence to be a human carcinogen. TDlinh applied to inhalation routes.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	Yes	Yes	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
		µg.kg-1.bw.d-1	Insufficient data with sufficient information on derivation to derive TDloral

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	Chloroethane evaluation summary last updated April 1999	20/04/2009	None presented	No data								
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>		20/04/2009	Links to many technical documents: no HCVs presented in limited nr documents read	No data								
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		20/04/2009	See Toxnet									
RBCA Toolkit chemical database	N/A	Model version 2.01	20/04/2009	RfD/TDSI oral	400	ug.kg-1.bw.d-1	400						
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/authorized.shtml">http://rais.ornl.gov/tox/authorized.shtml</a>	Jul-07	21/04/2009	p-SRfD i.e. provisional sub-chronic RfD.	100	ug.kg-1.bw.d-1	100	Low	NOAEL:	361	mg/kg d-1	3000	x10 for inter human variability, mouse to human extrapolation and database deficiencies. x3 for adjustment from 14 day study to sub chronic RfD
	<a href="http://rais.ornl.gov/tox/authorized.shtml">http://rais.ornl.gov/tox/authorized.shtml</a>	Jul-07	21/04/2009	RfD	no data								
RAIS	<a href="http://rais.ornl.gov/homepage/rap_tool.shtml">http://rais.ornl.gov/homepage/rap_tool.shtml</a>	06-Apr-09	20/05/2009	RfD oral	0.4	mg/kg/d	400						
				RfD oral	0.1	mg/kg/d	100	Provisional value					
Texas Commission on Environmental Quality	Texas: <a href="http://www.tceq.state.tx.us/remedia">http://www.tceq.state.tx.us/remedia</a>	25-Mar-09	20/05/2009	RfD oral	0.4	mg/kg/d	400						

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**Chloroethane**


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TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
International Agency for Research on Cancer (IARC)				Not classifiable as human carcinogen (IARC) <a href="http://www.inchem.org/documents/iarc/vol71/075-chlorethane.html">http://www.inchem.org/documents/iarc/vol71/075-chlorethane.html</a> : Group 3 classification (The agent (mixture or exposure circumstance) is not classifiable as to its carcinogenicity to humans)	
International Programme on Chemical Safety (IPCS)					
USEPA Integrated Risk Information System (IRIS)					
RBCA Toolkit chemical database		Source information not presented	Information not presented	US EPA National Center for Environmental Assessment (NCEA)	
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Sub chronic	Rat study (Dow 1995); 14 day duration		Provisional Peer Reviewed Toxicity Values for Chloroethane, Superfund Health Risk Technical Support Center, National Center for Environmental Assessment, USEPA. 24/7/2007	none
		The existing database does not support the development of a chronic oral p-RFD because of the lack of 90 day chronic oral studies.			none
RAIS	Chronic			USEPA Region 9 /NCEA (National Centre for Environmental Assessment)	?????
	Sub chronic				????
Texas Commission on Environmental Quality				Texas Risk Reduction Program, Toxicity and physical/chemical properties tables dated March 25, 2009	<a href="http://www.tceq.state.tx.us/assets/public/mediation/trrp/trrptoxchph_032509.xls">http://www.tceq.state.tx.us/assets/public/mediation/trrp/trrptoxchph_032509.xls</a>

Chloroethane	CAS Number: 75-00-3	Assessor A: Jane Thrasher (Jacobs)	Assessor B: Andy Singleton (ESI)	Final review: Panel/SF
		Date: 29/04/2009	Date: 30/04/2009	Date: 26/08/2009

TDI inhal	Recommended TDIinhal	Units	Justification
	2857	µg.kg-1.bw d-1	Adopt RfC of 10 mg/m3 (IRIS); adjusted to account for inhalation rate of 20 m3/d and 70kg body weight

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	EH40(2007 amendments)	15/04/2009	WEL and MEL	WEL: 134 (8 hr TWA) MEL: 50 (8 hr TWA)	mg/m3 ppm							
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>		20/04/2009	MRL (Minimal Risk Level); acute exposure	15 40	ppm mg/m3							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	04/01/1991	20/04/2009	RfC	10	mg/m3	2857	Medium	NOAEL LOAEL	4000 13000	mg/m3 mg/m3	300	A factor of 10 is used to account for sensitive populations. An uncertainty factor of 3 (rather than 10) is used for interspecies extrapolation due to dosimetric adjustment of the inhaled concentration. As no multigeneration reproductive study and no definitive developmental toxicity studies were available, a full factor of 10 is proposed for database deficiencies.
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	RfC verified 20/12/1990	20/04/2009	TLV (Threshold Limit Value)	100 260	ppm mg/m3							
				PEL (Permissible Exposure Limit)	1000 2600	ppm mg/m3							
				IDLH (Immediately Dangerous to Life or Health)	3800 10200	ppm mg/m3							
				RfC	10	mg/m3		Medium	NOAEL LOAEL	4000 13000	mg/m3 mg/m3	300	A factor of 10 is used to account for sensitive populations. An uncertainty factor of 3 (rather than 10) is used for interspecies extrapolation due to dosimetric adjustment of the inhaled concentration
RBCA Toolkit chemical database	N/A	Model version 2.01	20/04/2009	RfC/TCA	10	mg/m3							
RISC 4 chemical database		Version 4.05	20/04/2009	RfC/slope factor	N/D								
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Jul-07	21/04/2009	p-SRfC	4	mg/m3		Medium	BMD/LEC	1078	mg/m3	300	
US Army Corps	<a href="http://el.erd.c.usace.army.mil/arams/">US Army corps: http://el.erd.c.usace.army.mil/arams/</a>		20/05/2009	RfD inhal	2.86	mg/kg/d							
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rr.html">Texas: http://www.tceq.state.tx.us/remediation/rr.html</a>	25-Mar-09	20/05/2009	RfC	10	mg/m3							

## Chloroethane

Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Health and Safety Executive (HSE)	Information not available	WEL: workplace exposure limit MEL: maximum exposure limit		EH40(2007 amendments)	<a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a> <a href="http://www.hse.gov.uk/ria/chemical/chloroethane.pdf">http://www.hse.gov.uk/ria/chemical/chloroethane.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Derived from same study as RfC (see below)				<a href="http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf">http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Mouse developmental inhalation study in CF-1 mice	In a developmental study conducted in groups of 30 CF-1 mice, Scortichini et al. (1986) exposed animals to mean time-weighted averages of 0 (air), 491 +/-37 ppm (1.3 g/cu.m), 1504 +/- 84 ppm (4000 mg/cu.m), and 4946 +/- 159 ppm (13,000 mg/cu.m.) 99.9% ethyl chloride for 6 hours/day on days 6 through 15 of gestation. The animals were sacrificed on the 18th day of gestation. This study shows that exposure to ethyl chloride results in fetotoxicity. The exposure concentration of 1504 ppm is the NOAEL of this study NOAEL(HEC) = 4000 mg/cu.m based on foramina of the skull bones. The highest concentration used in this study, 4946 ppm, is a LOAEL, (HEC) = 13,000 mg/cu.m.	Delayed fetal ossification	Scortichini, B.H., K.A. Johnson, J.J. Momany-Pfruender, and T.R. Hanley, Jr. 1986. Ethyl chloride: Inhalation teratology study in CF-1 mice. Dow Chemical Co. EPA Document #86-870002248. 1986. US EPA IRIS Listing for Ethyl chloride (CASRN 75-00-3)	<a href="http://www.epa.gov/iris/subst/0523.htm">http://www.epa.gov/iris/subst/0523.htm</a>
Toxicology Data Network (Toxnet)	Information not available				
	Information not available				
	Information not available				
	30 CF-1 mice; chronic	Mouse study (Scortichini et al. 1986); 6-15 day duration	Delayed fetal ossification		<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search">http://toxnet.nlm.nih.gov/cgi-bin/sis/search</a>
RBCA Toolkit chemical database	Information not available			USEPA Integrated Risk Information System( IRIS), as of March 31, 2007	
RISC 4 chemical database					
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Sub chronic	Mouse study (Scortichini et al. 1986); 6-15 day duration	Delayed fetal ossification		
US Army Corps	Information not available	Value cited in ARAMS database (Adaptive Risk Assessment Modelling System); derived from IRIS		USEPA Integrated Risk Information System( IRIS)	
Texas Commission on Environmental Quality	Information not available			Texas Risk Reduction Program, Toxicity and physical/chemical properties tables dated March 25, 2009	<a href="http://www.tceq.state.tx.us/assets/public/mediation/trrp/trrptoxchph_032509.xls">http://www.tceq.state.tx.us/assets/public/mediation/trrp/trrptoxchph_032509.xls</a>

<b>Chloroethane</b>	CAS: 75-00-3	Assessor A: Jane Thrasher (Jacobs)	Assessor B: Andy Singleton (ESI)	Final review: Panel/SF
		Date: 29/04/2009	Date: 30/04/2009	Date: 26/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No literature data available for background exposures (note: gaseous in nature - minimal oral intake anticipated)
	0	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Assume 13.5µd/day in absence of any reliable UK data. Only literature value relates to US research from 1980.
	13.5	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Toxicological Data Network (TOXNET)	20/04/2009	Air intake	2.4 to 13.5 ug/day (average)	ug/day	Based on monitoring of four US cities in 1980.	Singh HB et al; Atmospheric Measurements of Selected Hazardous Organic Chemicals. USEPA-600/S3-81-032 p. 4-5 (1981)] PEER REVIEWED	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+75-00-3">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/r?dbs+hsdb:@term+@rn+75-00-3</a>

Substance:	<b>Chloroethane</b>	CAS Number:	75-00-3	Assessor A:	Jane Thrasher (Jacobs)	Assessor B:	Andy Singleton (ES)	Final review:	Panel/SF
Chemical Formula:	<b>C2H5Cl</b>	Phase at Ambient Temperature	Gas (volatile liquid at low temp)	Date:	29-Apr-09	Date:	30-Apr-09	Date:	26-Aug-09

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oecd.org/scripts/hgv/>

Property	Units	Calculated Value	Adopted value	Ref. Temp (C)	Rationale	References	Sources																											
							A HOWARD, 1990			B UDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000						
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)				
<b>Required Parameters</b>																																		
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	<b>64.51</b>	n/a	Agreed literature value		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)				
							Average	64.52	64.52	n/a	64.514	64.514	n/a	64.514	64.514	n/a	64.51	64.51	n/a	#VALUE!	#VALUE!	n/a	#VALUE!	#VALUE!	n/a	64.5138	64.5138	n/a	64.5138	64.5138	n/a			
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	<b>1.02E+03</b>	25	no consistent range - most recent value		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)				
							Geomean	8.48E-03	8.59E+02	25	1.02E+00	1.02E+03	25	2.50E+01	8.60E+02	860	n/a	n/a	n/a	1.11E-02	1.124.7075	25	No data	#VALUE!	n/a	8.40E-02	1.19E+03	n/a	8.82E-03	893.6865	24.8			
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	<b>5.74E+03</b>	10	Value chosen at 10 degrees		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	
							Geomean	5.71E+03	5.71E+03	20	Insert Values	Insert Values	20	5.74E+03	5.74E+03	10	5.74E+03	5.74E+03	20	5.71E+03	5.71E+03	20	No data	#VALUE!	n/a	Insert Values	Insert Values	20	4.50E+03	5.80E+03	20			
Chemical Boiling Point (ambient pressure)	K	n/a	<b>2.85E+02</b>	n/a	Consensus value		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	
							Average	12.3	285.45	n/a	12.3	285.45	n/a	12.3	285.45	n/a	12.3	285.45	n/a	12.3	285.45	n/a	No data	#VALUE!	n/a	289	289.00	n/a	12.3	285.45	n/a	n/a	n/a	
Chemical Melting Point (ambient pressure)	K	n/a	<b>1.35E+02</b>	n/a	Median value from consistent range of average values associated with individual references		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	
							Average	-138.7	134.45	n/a	-138.4	134.75	n/a	-138.4	134.75	n/a	-138.7	134.45	n/a	-136.4	136.75	n/a	No data	#VALUE!	n/a	132.3	132.30	n/a	-138.3	134.85	n/a	-136.4	136.75	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	<b>1.44</b>	n/a	Median value from consistent range of average values associated with individual references		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	
							Average	1.43	1.43	n/a	1.43	1.43	n/a	1.43	1.43	n/a	no data	no data	n/a	1.43	1.43	n/a	No data	No data	n/a	1.38	1.38	n/a	1.52	1.52	n/a	1.43	1.43	n/a
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	<b>7.27E+01</b>	n/a	Single value		n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
							Average						72.7	72.70	n/a																			
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	24650.34574	<b>2.47E+04</b>	n/a	Normal Chemical Boiling Point		n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
							Average	24.65	24650	n/a	24.652	24652	n/a	24.652	24652	n/a	24.652	24652	n/a	24.652	24652	n/a	24.652	24652	n/a	24.652	24652	285.42	24.652	24652	285.42	24.652	24652	
Chemical Critical Point temperature (ambient pressure)	K	459.7656709	<b>459.8</b>	n/a	Calculated value chosen - this is consistent to range of reported values		n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							Average	460.4	460.40	n/a	460.4	460.40	n/a	460.4	460.40	n/a	187.2	460.35	n/a	460.3	460.30	n/a	460.3	460.30	n/a	460.3	460.30	n/a	460.3	460.30	n/a	460.3	460.30	n/a
Critical Pressure	atm	51.98243991	<b>51.98</b>	n/a	Calculated value chosen - this is consistent to range of reported values		n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							Average	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	n/a	53	52.30693314	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	4.451E-01	10	Estimated from parameters above using Claypyron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	93271.64765	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	1.05E-05	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	7.83E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	1.27	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Chloromethane / Methyl Chloride	CAS Number:	74-87-3	Assessor A:	A. Fellows	Assessor B:	S. Cole	Final review:	Panel/SF
	Date	28.05.2009	Date	26.06.2009	Date	09/09/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	NR	Group 3 carcinogen (IARC), no strong evidence to be a human carcinogen - Insufficient data to derive TDloral
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	Yes	Yes	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
		ug.kg-1.d-1	Insufficient data with required supporting data to derive a TDlinhal (USEPA Health Advisors RfD based on IRIS RfD which has subsequently been withdrawn)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	19/02/2000	27/05/2009	Data In German									
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/dinking">http://www.epa.gov/waterscience/criteria/dinking</a>	Published drinking water health advisory August 2006, based on chloromethane report 1989	28/05/2009	RfD	0.004	mg/kg/day	4	Unknown		0.004	mg kg day	unknown	unknown
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	July 2001	28/05/2009	Methyl chloride exists primarily as a gas. No adequate oral exposure studies exist from which an oral RfD may be derived.									

TDI inhal	Recommended TDlinhal	Units	Justification
	5.14	ug.kg-1.d-1	CICADs TDI used as this is most conservative

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	2000	27/05/2009	TDI	0.00514	mg kg day	5.14	Unknown	LOAEL	18	mg/m3	1000	10 for intraspecies variability, 10 for interspecies variation and 10 for poor database and LOAEL use.
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	<a href="http://inchem.org/pages/sids.html">http://inchem.org/pages/sids.html</a>	2002	27/05/2009	TDI	1.2857	mg kg day	1285.7	Unknown	NOAEL	450	mg/m3	100	10 for intraspecies variability, 10 for interspecies variation. (Unknown, applied).
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	December 1998	28/05/2009	MRL	0.05 (0.028571)	ppm (mg kg day)	28.57	Unknown	LOAEL	51	ppm	1000	10 for intraspecies variability, 10 for interspecies variation and 10 for LOAEL

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**Chloromethane / Methyl Chloride**


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**TDI oral**


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Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
European Chemicals Bureau (ECB)					
USEPA Health Advisors	unknown	Compilation Table 2006 drinking water standards and health advisories. Stated Reference Dose for Oral consumption of water. RfD quoted from IRIS in report.	unknown	Drinking water standards. Page 8 in source.	<a href="http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf">http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf</a>
USEPA Integrated Risk Information System (IRIS)					<a href="http://www.epa.gov/iris/subst/1003.htm">http://www.epa.gov/iris/subst/1003.htm</a>

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**TDI inhal**


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Organisation	Study type	Description	Response	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)	Fischer 344 Rats and B6C3F1 Mice Chronic	Two year inhalation study of rats and mice. (CIIT, 1981). 103mg/m3 LOAEL converted for continuous exposure to 18 mg/m3. (0.0018 mg/m3 reported as guidance value for indirect exposure via environment)	Exposure at LOAEL of 103 mg/m3 (50 ppm) induced Axonal swelling and degeneration of spinal nerves. Also supported by renal microcysts in 103 mg/m3 group	Chemical Industry Institute of Toxicology. Final report on a chronic inhalation toxicology study in rats and mice exposed to methyl chloride. Unpublished study prepared by Battelle-Columbus Laboratories, Columbus, OH. OTS Submission Document ID 40-8120717. Microfiche No. 511310. (1981).	<a href="http://www.inchem.org/documents/cicads/cicads/cicad28.htm">http://www.inchem.org/documents/cicads/cicads/cicad28.htm</a>
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	Fischer 344 Rats and B6C3F1 Mice Chronic	Two year inhalation bioassay rats and mice exposed to 100, 450, 2000 mg/m3.	Exposure at LOAEL of 2000 mg/m3 increased heart weights, kidney and liver weights in rats. Severe effects were seen in mice at the LOAEL.	SIDS Initial Assessment Report for SIAM 15 (Boston, USA, October 2002)	<a href="http://www.inchem.org/documents/sids/sids/CLMETHANE.pdf">http://www.inchem.org/documents/sids/sids/CLMETHANE.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Mouse B6C3F1 Chronic	18 month inhalation study used in derivation of inhalation MRL	axonal swelling and slight degeneration of axons in spinal cord.	Toxicological profile for chloromethane December 1998 Section 2 and section 7. From study by CIIT 1981	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp106.html">http://www.atsdr.cdc.gov/toxprofiles/tp106.html</a>

Chloromethane / Methyl Chloride		CAS Number:	74-87-3		Assessor A:	A. Fellows		Assessor B:	S. Cole		Final review:	Panel/SF	
					Date	28.05.2009		Date	26.06.2009		Date	09/09/2009	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	Study 1983, 1985 (Last revised on website 17/07/2001)	26/05/2009	RfC	0.09	mg/m <sup>3</sup>	25.71	Medium	NOAEL	94.6	mg / m3	1000	A factor of 3 for interspecies extrapolation, 10 for extrapolation from an 11 day study to a lifetime study and a factor of 10 for intraspecies variability and lack of brain histopathology in F1 mice. Because two factors of 3 (101/2) coalesce to a 10, the total uncertainty factor applied to NOAEL the of 94.6 mg/m3 is 1,000

ID oral				Recommended IDoral	Units	Justification
				n/a		IARC classification: Group 3, insufficient evidence for the carcinogenicity of methyl chloride to humans, 1999. IRIS classification: Group D, not classifiable as t

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	13/04/1999	27/05/2009							"There is inadequate evidence for the carcinogenicity of Methyl Chloride to humans."
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	07/17/2001	28-May-09							Data for carcinogenicity in humans is considered inadequate. methyl chloride is most appropriately designated a Group D - Not classifiable as to its human carcinogenicity.

ID inhal				Recommended IDinhal	Units	Justification
				n/a		IARC classification: Group 3, insufficient evidence for the carcinogenicity of methyl chloride to humans, 1999. IRIS classification: Group D, not classifiable as t

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	13/04/1999	27/05/2009							"There is inadequate evidence for the carcinogenicity of Methyl Chloride to humans."
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	07/17/2001	28-May-09							Data for carcinogenicity in humans is considered inadequate. methyl chloride is most appropriately designated a Group D - Not classifiable as to its human carcinogenicity.

**Chloromethane / Methyl Chloride**

USEPA Integrated Risk Information System (IRIS)	Mouse Intermediate	11 Day Mouse inhalation study	cerebellar lesions	IRIS Database - Landry et al., 1983, 1985	<a href="http://www.epa.gov/NCEA/iris/subst/1003.htm">http://www.epa.gov/NCEA/iris/subst/1003.htm</a> <a href="http://www.epa.gov/ncea/iris/toxreviews/1003-tr.pdf">http://www.epa.gov/ncea/iris/toxreviews/1003-tr.pdf</a>
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**ID oral**

o its human carcinogenicity (2001).

Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)		Methyl Chloride is not classifiable as to its carcinogenicity to humans (Group 3)		International Agency for Research on Cancer (IARC) - Summaries & Evaluations. Vol 71. (1999) p. 737.	<a href="http://www.inchem.org/documents/iarc/vol71/026-methylchloride.html">http://www.inchem.org/documents/iarc/vol71/026-methylchloride.html</a>
USEPA Integrated Risk Information System (IRIS)					<a href="http://www.epa.gov/iris/subst/1003.htm">http://www.epa.gov/iris/subst/1003.htm</a>

**ID inhal**

o its human carcinogenicity (2001).

Organisation	Study type	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)		Methyl Chloride is not classifiable as to its carcinogenicity to humans (Group 3)		International Agency for Research on Cancer (IARC) - Summaries & Evaluations. Vol 71. (1999) p. 737.	<a href="http://www.inchem.org/documents/iarc/vol71/026-methylchloride.html">http://www.inchem.org/documents/iarc/vol71/026-methylchloride.html</a>
USEPA Integrated Risk Information System (IRIS)					<a href="http://www.epa.gov/iris/subst/1003.htm">http://www.epa.gov/iris/subst/1003.htm</a>

<b>Chloromethane</b>	CAS 74-87-3	Assessor A:	A. Fellows	Assessor B:	S. Cole	Final review:	Panel/SF
		Date	28/05/2009	Date	26.06.2009	Date	09/09/2009

<b>MDI</b>	<b>Recommend ed MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No suitable data on likely average exposure. Chloromethane exists primarily as a gas, therefore reasonable to assume background oral concentration is negligible.
	<b>0</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	22/06/1905	Surface Water - River Rhine	12	ug/l	maximum concentration in surface waters of Europe - River Rhine	Concise International Chemical Assessment Document 28. page 10	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	22/06/1905	Drinking water well	44	ug/l	maximum concentration of drinking water well in USA	Concise International Chemical Assessment Document 28. page 10	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Organisation for the Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	22/10/2002	water	0.222	ug/l	Observed at low concentrations in water (No reference stated)	SIDS Initial Assessment Profile. (SIAM 15)	<a href="http://inchem.org/pages/sids.html">http://inchem.org/pages/sids.html</a>

<b>MDI</b>	<b>Recommend ed MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Average urban concentration from all reported values (IPCS CICAD data). Adjusted for CLEA adult inhalation assuming inhalation of 20m <sup>3</sup> /day.
	<b>212</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	2000	outdoor air concentrations in urban environments	10.62	ug/m <sup>3</sup>	Measured Air concentrations in urban/suburban USA, three Japanese cities, Delft (Netherlands) and Lisbon (Portugal).	Concise International Chemical Assessment Document 28. page 9	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>
Organisation for the Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	22/10/2002	ambient air	700	ppt	Natural levels of Chloromethane in ambient air	SIDS Initial Assessment Profile. (SIAM 15)	<a href="http://inchem.org/pages/sids.html">http://inchem.org/pages/sids.html</a>



Cis 1,2 Dichloroethene	CAS Number:	156-59-2	Assessor A:	Nick Brown, Grontmij	Assessor B:	Catherine Helm, WD Environmental	Final Review:	Panel/SF
	Date	26/05/2009	Date	29/05/2009	Date	28/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to Exposure Routes ?	Yes	Yes	Yes	NR	EPA classifies Cis 1,2 Dichloroethene as D - not classifiable as to human carcinogenicity. Carcinogenicity data is generally absent. TDloral applied to oral and dermal routes
Apply IDoral to Exposure Routes ?	No	No	No		
Apply TDlinh to Exposure Routes ?	No	No	No		
Apply IDinhal to Exposure Routes ?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	6	ug/kg/day	RIVM health criterion selected as this is conservative and chemical specific (IPCS/JECFA is based on trans-isomer).

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	Published 2003	29/04/2009	TDI	17	ug/kg bw/day	17		NOAEL for trans isomer	17	mg/kg-bw-day	1000	10 each for inter- and intraspecies variation, 10 for limited study duration
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/iecfa/en/">http://who.int/ipcs/food/iecfa/en/</a>	Published 2003	29/04/2009	TDI	17	ug/kg bw/day	17		NOAEL for trans isomer	17	mg/kg-bw-day	1000	10 each for inter- and intraspecies variation, 10 for limited study duration
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001	29/04/2009	TDI Oral	6	ug/kg bw/day	6	Medium Reliability	NOAEL	32	mg/kg-bw/day	5000	10 each for inter- and intraspecies variation, 10 for limited study duration, and 5 for severity of endpoint
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Re-published 2008	29/04/2009	Oral Minimum Risk Level (int)	0.3	mg/kg bw/day	300		NOAEL	32	mg/kg-bw/day	100	x10 for inter- and x 10 for intraspecies variation
USEPA Acute Guideline Levels (AEGs)	<a href="http://epa.gov/oppt/aegl/pubs/chemlist.htm">http://epa.gov/oppt/aegl/pubs/chemlist.htm</a>		02/04/2009	8-hour AEGs	140, 230, 310	ppm	158, 259.6, 349.9						
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Published 2006		Chronic RfD	0.01	mg/kg bw/day	10	Low	NOAEL	32	mg/kg-bw/day	3000	10 each for inter- and intraspecies variation, 10 for limited study duration, and 3 for database limitations including lack of reproductive or developmental studies

TDI inhalation	Recommended TDlinhal	Units	Justification
		ug/kg/day	insufficient data with sufficient detail on derivation to derive. Use route-to-route extrapolation from oral. RIVM 'route to route extrapolation' method is unclear, value is 0

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001	29/04/2009	Preliminary TCA (tolerable concentration in air)	30	ug/m3	8.57	Low Reliability	Route to route extrapolation from the oral TDI			5000	10 each for inter- and intraspecies variation, 10 for limited study duration, and 5 for severity of endpoint

Cis 1,2 Dichloroethene

<b>TDI oral</b>
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Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
<b>International Programme on Chemical Safety (IPCS)</b>	Barnes 90 day CD1 mice study using the trans isomer	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Increased serum alkaline phosphate levels in males and decreased thymus weight in females. Human effects include CNS depression, neurological effects and trans is estimated to be 2x more potent than cis isomer	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72). Primary study - Barnes DW et al. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chemistry and toxicology, 1985, 8:373-407	<a href="http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf</a>
<b>Joint Expert Committee on Food Additives (JECFA)</b>	Barnes 90 day CD1 mice study using the trans isomer	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Increased serum alkaline phosphate levels in males and decreased thymus weight in females. Human effects include CNS depression, neurological effects and trans is estimated to be 2x more potent than cis isomer	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72) Primary study - Barnes DW et al. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chemistry and toxicology, 1985, 8:373-407	<a href="http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf</a>
<b>Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels</b>	Macauley 90 day rat study	Semi-chronic study on rats. Dose groups included male and females at 97 and 290 mg/kg-bw/day - reductions in haemoglobin and haemocrit recorded at these concentrations. 32mg/kg-bw/day identified as a NOAEL	haematopoietic system effects	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001 (McCauley PT et al. 1995. The effect of subacute and subchronic oral exposure to cis-1,2-dichloroethylene in Sprague-Dawley rats. Drug Chem Toxicol 18, 171-184.)	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
<b>US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels</b>	Macauley 90 day rat study	Semi-chronic study on rats. Dose groups included male and females at 97 and 290 mg/kg-bw/day - reductions in haemoglobin and haemocrit recorded at these concentrations. 32mg/kg-bw/day identified as a NOAEL	Haematological	ATSDR Minimum Risk Levels December 2008 and Toxicological Profile for 1,2-Dichloroethene, ATSDR, 1996 available at <a href="http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf</a> (Primary Reference for the Study: Macauley et al. 1990. The effects of subacute and subchronic oral exposure to Cis-1,2-dichloroethylene in Rats. Human Effects Research Laboratory, U.S. EPA, Cincinnati, OH and Air Force Aerospace Medical Research Laboratory, Wright-Patterson AFB, OH)	<a href="http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf">http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf</a>
<b>USEPA Acute Guideline Levels (AEGs)</b>					
<b>US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)</b>	Macauley 90 day rat study	Semi-chronic study on rats. Dose groups included male and females at 97 and 290 mg/kg-bw/day - reductions in haemoglobin and haemocrit recorded at these concentrations. 32mg/kg-bw/day identified as a NOAEL	Mild Anemic Changes	Provisional Peer Reviewed Toxicity Values for cis-1,2-dichloroethylene, Superfund Health Risk Technical Support Centre for Environmental Assessment, 2006. EPA Health Effects Assessment Summary Table (HEAST) cited as source of the RfD. (Primary Reference for the Study: Macauley et al. 1990. The effects of subacute and subchronic oral exposure to Cis-1,2-dichloroethylene in Rats. Human Effects Research Laboratory, U.S. EPA, Cincinnati, OH and Air Force Aerospace Medical Research Laboratory, Wright-Patterson AFB, OH)	

<b>TDI inhalation</b>
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nly provisional and therefore more stringent RIVM oral TDI is considered appropriate.

Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
<b>Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels</b>	Extrapolation from ORAL TDI based on Macauley 90 day rat study	Extrapolation from ORAL TDI based on 90 day rat study	critical effects of oral intake were haematopoietic system effects	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001 (McCauley PT et al. 1995. The effect of subacute and subchronic oral exposure to cis-1,2-dichloroethylene in Sprague-Dawley rats. Drug Chem Toxicol 18, 171-184.)	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>

<b>Cis-1,2-dichloroethene</b>	CAS 156-59-2	Assessor A:	Nick Brown Grontmij	Assessor B:	Catherine Helm WD Environmental	Final Review	Panel/SF
		Date	29/05/2009	Date	01/06/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDIoral</b>	<b>Units</b>	<b>Justification:</b> Only US Data has been identified. In the majority of cases exposure through drinking water and food is likely to be negligible however sources in drinking water have been identified. A value of 4ug day-1 for background exposure through drinking water is tentatively proposed within the WHO Background document for development of WHO Guidelines for Drinking Water Quality. This value appears to be based on the US study that identified detectable concentrations in 8% of drinking water sources with detectable concentrations ranging between 2-120ug/l. In conjunction with the MDI Inhalation (6ug day-1 see below) this equates to a total of 10ug/day background exposure which conforms reasonably well with the RIVM estimate of total background exposure to the mixed isomers of 0.13ug/kg-bw/day (9.1ug/day for a 70kg adult). The same value has also been selected for the trans isomer since the primary study does not distinguish between the two isomers.
	4	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
International Programme on Chemical Safety (IPCS)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>
Joint Expert Committee on Food Additives (JECFA)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>
WHO Guidelines for Drinking Water Quality	14/04/2009	Drinking water	4	ug/day	1,2 dichloroethene (mixed isomers) detected in 8% of drinking supplies derived from groundwater, at concentrations between 2-120ug/l. The high end value is therefore greatly atypical with the majority of drinking water containing concentrations less than detection levels. Estimated 4ug/l MDI is based on a concentration of 2ug/l in drinking water.	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Drinking water	0-120	ug/l	Dutch data not available. 1,2 dichloroethene (mixed isomers) detected in 8% of drinking supplies derived from groundwater, at concentrations between 2-120ug/l. RIVM estimated background exposure of 0.13ug/kg-bw/day for the mixed isomers via inhalation and oral intake.	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Drinking water	0-120	ug/l	1,2 dichloroethene (mixed isomers) detected in 8% of drinking supplies derived from groundwater, at concentrations between 2-120ug/l. The high end value is atypical with the majority of drinking water containing concentrations less than detection levels.	Toxicological Profile for 1,2-Dichloroethene, ATSDR, 1996	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf</a>
USEPA Health Advisories	14/04/2009	DW	0.07	mg/l	MCLG & MCL		<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
Toxicological Data Network (TOXNET)	14/04/2009		ND to 408	ug/l	ADI from water in HSDB Database (Cis isomer specific)	(3) EPA; National Contaminant Occurrence Database. cis-1,2-Dichloroethylene. Available from the Database Query page at <a href="http://www.epa.gov/safewater/data/ncod.html">http://www.epa.gov/safewater/data/ncod.html</a> as of Apr 12, 2001.	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
<b>MDI</b>	<b>Recommended MDIinh</b>	<b>Units</b>	<b>Justification:</b> Only US Data has been identified. The value of 6ug/day is the maximum value within range that ATSDR suggest that the general US population is likely to be exposed to. In conjunction with the MDI Oral (4ug day-1 see above) this equates to a total of 10ug/day background exposure which conforms reasonably well with the RIVM estimate of total background exposure to the mixed isomers of 0.13ug/kg-bw/day (9.1ug/day for a 70kg adult). The same value has also been selected for the trans isomer since ATSDR do not distinguish between the two isomers.				
	6	ug day-1					

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Joint Expert Committee on Food Additives (JECFA)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>
WHO Guidelines for Drinking Water Quality	14/04/2009	Urban and suburban air - Cis isomer	644 (Based on 20m3 x 32.2ug/m3)	ug/day	1,2 Dichloroethene (mixed isomers) recorded at mean concentrations of 32.2ug/m3 within indoor air (Data source unclear). Mean concentrations of the Cis isomer recorded in the range 0.04-0.3ug/m3 in urban and industrial areas.	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Urban and suburban air - Cis isomer	0.27	ug/m3	Dutch data not available. Average air concentration of the Cis isomer of 0.27ug/m3 recorded in urban and suburban air in US study. RIVM estimated background exposure of 0.13ug/kg-bw/day for the mixed isomers via inhalation and oral intake.	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Ambient air	6	ug/day	The general population (USA) estimated to be exposed to low levels of 1,2 dichloroethene (mixed isomers) through inhalation in urban air (1-6ug/day)	Toxicological Profile for 1,2-Dichloroethene, ATSDR, 1996	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf</a>
Toxicological Data Network (TOXNET)	14/04/2009	Air	0.068-0.326	ppb	ADI from air in HSDB Database	1) Shah JJ, Singh HB; Environ Sci Technol 22: 1381-1388 (1988) (2) EPA; Volatile organic chemicals in the atmosphere: An assessment of available data. Menlo Park, CA: SRI Int p. 198 (1982) EPA-600/3-83-027A	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

Substance:		Cis 1,2 Dichloroethene		CAS Number: 156-59-2		Assessor A: Claire Potter		Assessor B: Catherine Heim		Final Review: Panel/SF																							
Chemical Formula:		C2H2Cl2		Phase at Ambient Temperature: Liquid		Date: 01-Apr-09		Date: 29/05/2009		Date: 28/08/2009																							
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H					
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																																	
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	96.94	n/a	Median value from consistent range of literature values	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
							96.94	96.94	n/a	96.943	96.943	n/a	96.943	96.943	n/a	96.94	96.94	n/a	96.94	96.94	n/a	96.94	96.94	n/a	96.9427	96.9427	n/a	96.9427	96.9427	n/a	96.9427	96.9427	n/a
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	4.60E+02	25	Adopted value is that from the newest source (Lide 2008) as there is no consistent range	Geomean	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	KPa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	Pa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)
							3.37E-03	3.41E+02	25	4.60E-01	4.60E+02	25	3.42E+02	342.2	745.5	745.5	745.5	745.5	9.09E-03	921.04425	25	2.40E-01	4.18E+02	25	2.40E-01	4.18E+02	25	2.40E-01	4.18E+02	25	2.40E-01	4.18E+02	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	7.55E+03	10	Median of three literature values which show consistent range at 10 degrees	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
							3.50E+03	3.50E+03	n/a	7.60E+00	7600	10	3.52E+03	3.52E+03	25	3.52E+03	3.52E+03	25	6.26E+03	6.26E+03	25	6.26E+03	6.26E+03	25	6.26E+03	6.26E+03	25	6.26E+03	6.26E+03	25	6.26E+03	6.26E+03	25
Chemical Boiling Point (ambient pressure)	K	n/a	3.33E+02	n/a	Median value from consistent range of literature values	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							60.3	333.45	n/a	60.1	333.25	n/a	60.1	333.25	n/a	59.6	332.75	n/a	47.5	320.65	n/a	333.34	333.34	n/a	333.34	333.34	n/a	333.34	333.34	n/a	333.34	333.34	n/a
Chemical Melting Point (ambient pressure)	K	n/a	1.93E+02	n/a	Median value from consistent range of values	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							-80.5	192.65	n/a	-80	193.15	n/a	-80	193.15	n/a	-81.5	191.65	n/a	-50	223.15	n/a	193	193.00	n/a	193	193.00	n/a	193	193.00	n/a	193	193.00	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	1.86	n/a	Median value from consistent range of values	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
							1.86	1.86	n/a	1.86	1.86	n/a	1.86	1.86	n/a	1.86	1.86	n/a	2.06	2.09	n/a	2.06	2.09	n/a	2.06	2.09	n/a	2.06	2.09	n/a	2.06	2.09	n/a
Molar Volume (Le Bas method)	cm3 mol <sup>-1</sup>	n/a	8.62E+01	n/a	Single available value	Average	n/a	n/a	n/a	n/a	n/a	n/a	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
													86.2	86.20	n/a																		
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	29732.73616	2.97E+04	Normal Chemical Boiling Point	Calculated Value	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
													30.2	30200	Normal Boiling Point	31.57	31570	Normal Boiling Point	30.23	30230	Normal Boiling Point	29	29000	Normal Boiling Point	33	33000	Normal Boiling Point	30.9	30900	Normal Boiling Point			
Chemical Critical Point temperature (ambient pressure)	K	526.8153773	5.27E+02	n/a	Calculated Value	Average	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
													544.2	544.20	n/a																		
Critical Pressure	atm	51.19955043	51.20	n/a	Calculated Value	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale	Property	Units	Calculated Value	Ref. Temp (C)	Rationale	Property	Units	Calculated Value	Ref. Temp (C)	Rationale	Property	Units	Calculated Value	Ref. Temp (C)	Rationale					
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	7.461E-02	10	Estimated from parameters above using Claypyon relationship or direct calculation	Vapour pressure at ambient soil temperature	Pa	13685.6591	10	Estimated from parameters above using Grain-Watson method	Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	9.02E-06	10	Estimated from parameters above using Wilkie-Lee method	Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	7.08E-10	10	Estimated from parameters above using Hayduk and Laudie method	Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	1.61	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Dichloromethane

CAS Number:	75-09-2	Assessor A:	Nick Brown, Grontmij	Assessor B:	Catherine Helm, WD Environmental	Final Review:	Panel/SF
		Date:	26/05/2009	Date:	01-Jun-09	Date:	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Human studies are considered generally inadequate to demonstrate whether or not DCM is carcinogenic. See detailed discussion below regarding selection of threshold behaviour for dichloromethane. TDloral applied to oral and dermal routes.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	6	ug.kg-1.d-1	Based on NCA 1982 study, cited by WHO DW, IPCS, JECFA.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Health and Safety Laboratory (HSL)	<a href="http://www.hsl.gov.uk/">http://www.hsl.gov.uk/</a>		02/04/2009	8-hour time weighted average	100	ppm (1ppm = 3.5 mg/m3)	100000						
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	Data reviewed 2003	14/04/2009	DW guideline	6	ug/kg/day	6		NOAEL		6 mg/kg bw/day	1000	100 for intra and inter species variation and 10 for concern about carcinogenic potential
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/jecfa/en/">http://who.int/ipcs/food/jecfa/en/</a>	Published 2003	05/05/2009	TDI oral	6	ug/kg/day	6		NOAEL		6 mg/kg bw/day	1000	100 for intra and inter species variation and 10 reflecting concern about carcinogenic potential
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwa/guidelines/en">http://www.who.int/water_sanitation_health/dwa/guidelines/en</a>		02/04/2009	TDI oral	6	ug/kg/day	6		NOAEL		6 mg/kg bw/day	1000	100 for intra and inter species variation and 10 reflecting potential for carcinogenic potential
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001			60	ug/kg/day	60						
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>		01/04/2009	MRL	60	ug/kg/day	60		NOAEL		6 mg/kg bw/day	100	x 10 interspecies and x 10 intraspecies
USEPA Acute Guideline Levels (AEGs)	<a href="http://epa.gov/oppt/aegl/pubs/chemist.htm">http://epa.gov/oppt/aegl/pubs/chemist.htm</a>	13/11/2009	14/04/2009	AEGs	60 & 2100	ppm (1ppm = 3.5 mg/m3)	60000 and 2100000						
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/dri nking">http://www.epa.gov/waterscience/criteria/dri nking</a>	Summer 2006	14/04/2009	MCL	0.005	mg/l	0.14						
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		02/04/2009	RfD	60	ug/kg/day	60	High confidence in study. Medium Confidence in RfD	NOAEL			100	x 10 interspecies and x 10 intraspecies
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>		28/04/2009	See IRIS above	See IRIS above	See IRIS above	See IRIS above	See IRIS above	See IRIS above				See IRIS above

## Dichloromethane

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Health and Safety Laboratory (HSL)					
International Programme on Chemical Safety (IPCS)	Fischer 344 Rat study	2-year drinking water study in rats exposed to 0, 5, 50, 125 and 250mg/kg-bw/day for 104 weeks	Liver/ Hepatic histological alterations and fatty changes. LOAEL recorded at 52mg/kg-bw/day	NCA 1982. Dichloromethane in Drinking Water. Background to the Development of WHO Guidelines for Drinking Water Quality. WHO 2003 (First Published 1996) (Serota D, Thakur AK, Ulland BM, et al. 1986. A Two Year water study of dichloromethane in rodents. I. Rats. Food Chem Toxicol 24:951-958)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethanesum.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethanesum.pdf</a>
Joint Expert Committee on Food Additives (JECFA)	Fischer 344 Rat study	2-year drinking water study in rats exposed to 0, 5, 50, 125 and 250mg/kg-bw/day for 104 weeks	Liver/ Hepatic histological alterations and fatty changes. LOAEL recorded at 52mg/kg-bw/day	NCA 1982. Dichloromethane in Drinking Water. Background to the Development of WHO Guidelines for Drinking Water Quality. WHO 2003 (First Published 1996) (Serota D, Thakur AK, Ulland BM, et al. 1986. A Two Year water study of dichloromethane in rodents. I. Rats. Food Chem Toxicol 24:951-958)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf</a>
WHO Guidelines for drinking water Quality	Fischer 344 Rat study	2-year drinking water study in rats exposed to 0, 5, 50, 125 and 250mg/kg-bw/day for 104 weeks	Liver/ Hepatic histological alterations and fatty changes. LOAEL recorded at 52mg/kg-bw/day	NCA 1982. Dichloromethane in Drinking Water. Background to the Development of WHO Guidelines for Drinking Water Quality. WHO 2003 (First Published 1996) (Serota D, Thakur AK, Ulland BM, et al. 1986. A Two Year water study of dichloromethane in rodents. I. Rats. Food Chem Toxicol 24:951-958)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels				RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	Fischer 344 Rat study	85 rats/ sex at each of four nominal dose groups (i.e., 5, 50, 125 and 250 mg/kg/day) for 2 years. Many effects were monitored. Treatment related histological alterations of the liver were evident at nominal doses of 50 mg/kg/day or higher. The low nominal dose of 5 mg/kg/day was a NOAEL. Same study as WHO Guidelines for Drinking Water Quality	Liver	(Serota D, Thakur AK, Ulland BM, et al. 1986. A Two Year water study of dichloromethane in rodents. I. Rats. Food Chem Toxicol 24:951-958)	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp14-a.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp14-a.pdf</a>
USEPA Acute Guideline Levels (AEGs)					
USEPA Health Advisors					
USEPA Integrated Risk Information System (IRIS)	Fischer 344 Rat study	85 rats/ sex at each of four nominal dose groups (i.e., 5, 50, 125 and 250 mg/kg/day) for 2 years. Many effects were monitored. Treatment related histological alterations of the liver were evident at nominal doses of 50 mg/kg/day or higher. The low nominal dose of 5 mg/kg/day was a NOAEL. Same study as WHO Guidelines for Drinking Water Quality	Liver	National Coffee Association. 1982. 24-Month chronic toxicity and oncogenicity study of methylene chloride in rats. Final Report. Prepared by Hazleton Laboratories America, Inc., Vienna, VA. (Unpublished) (Serota D, Thakur AK, Ulland BM, et al. 1986. A Two Year water study of dichloromethane in rodents. I. Rats. Food Chem Toxicol 24:951-958)	<a href="http://www.epa.gov/NCEA/iris/subst/0070.htm">http://www.epa.gov/NCEA/iris/subst/0070.htm</a>
Toxicology Data Network (Toxnet)	See IRIS above	See IRIS above	See IRIS above	See IRIS above	See IRIS above

Dichloromethane	CAS Number: 75-09-2	Assessor A: Nick Brown, Grontmij	Assessor B: Catherine Helm, WD Environmental	Final Review: Panel/SF
	Date: 26/05/2009	Date: 01-Jun-09	Date: 28/08/2009	

<b>TDI inhal</b>	<b>Recommended TDIinhal</b>	<b>Units</b>	<b>Justification</b>
	134.3	ug.kg-1.d-1	Derived from WHO weekly average. WHO based on human study, most conservative value.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>		01/04/2009	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/jecfa/en/">http://who.int/ipcs/food/jecfa/en/</a>		02/04/2009	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO	As WHO
WHO Air Quality guidelines for Europe	<a href="http://www.euro.who.int/air/activities/20050222_2">http://www.euro.who.int/air/activities/20050222_2</a>		02/04/2009	Air Quality Guideline	3 (0.47 - weekly average)	mg/m3	857 (134.3)		Predicted to cause 1% increase in COHb			NA	NA
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001	02/04/2009	TCA	3000	ug/m3	857		WHO value adopted			NA	NA
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>		05/05/2009	MRL	0.3 (1.05)	ppm (mg/m3)	300		NOAEL				30 x 3 interspecies and x 10 intraspecies
ATSDR 2	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>		05/05/2009	Maximum concentration associated with acute exposure and irreversible harm	750	ppm							

<b>ID oral</b>	<b>Recommended IDoral</b>	<b>Units</b>	<b>Justification</b>
	N/A	ug.kg-1.d-1	Human studies are considered generally inadequate to demonstrate whether or not DCM is carcinogenic, however, carcinogenicity has been demonstrated in mice and to a lesser extent in female rats. IRIS provides the carcinogenic Classification —B2; probable human carcinogen. IARC classified dichloromethane as possibly carcinogenic to humans (Group 2B), based on inadequate evidence for the carcinogenicity of dichloromethane in humans and sufficient evidence for the carcinogenicity of dichloromethane in experimental animals. Health Canada classified dichloromethane as "probably carcinogenic to humans" (Group II) and has generated PBK modified TD05 values (5% incidence of tumours). IRIS has also quantified carcinogenic risk by predicting concentrations equivalent to increased cancer risk of E-5. In relation to the tendency for tumor development in mice through exposure to DCM by inhalation, TERA comment that; "there are clear species differences in the putatively carcinogenic pathway of metabolism of dichloromethane which are consistent with the hypothesis that humans are likely to be less sensitive than some species of experimental animals in this regard". RIVM determined that dichloromethane is not considered to be genotoxic to humans, and therefore, derived risk values based on a threshold approach. Threshold based HCVs are also provided by ATSDR and WHO.  In view of the uncertainty remaining in relation to the actual carcinogenicity of DCM to humans and uncertainty relating to the methods of quantification of non-threshold risk, particularly in view of the guidance provided within SR2, the selection of conservative TDIs is considered more appropriate at this stage than the derivation Index Doses.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		02/04/2009			Carcinogenic risk level of E-5		50 ug/l		1.42 Extrapolation Method — Linearized multistage procedure, extra risk
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>		02/04/2009	Yes			See IRIS data	See IRIS data	See IRIS data	See IRIS data

## Dichloromethane

TDI inhal					
Organisation	Study type	Description	Response	Reference	Web link
International Programme on Chemical Safety (IPCS)	As WHO	As WHO	As WHO	As WHO	As WHO
Joint Expert Committee on Food Additives (JECFA)	As WHO	As WHO	As WHO	As WHO	As WHO
WHO Air Quality guidelines for Europe	Linear extrapolation from Divecenco and Kaplan (1981) - Human study of vapour intake	Humans exposed to doses between 175 700mg/m <sup>3</sup> for 7.5 hours - exhaled vapours were analysed to allow estimation of biotransformation	Critical effect linked to the accumulation of carboxyhaemoglobin (COHb) to unsafe levels (3%). The recommended value of 3mg/m <sup>3</sup> is predicted to cause a 0.1% increase in COHb	WHO Regional Office for Europe, Copenhagen, Denmark. 2000, Air Quality Guidelines 2nd Edition Primary study reference: Divecenco GD and Kaplan CJ (1981): Effect of exercise or smoking on the uptake, metabolism and excretion of methylene chloride vapour by humans. Toxicol Appl Pharmacol 59, 141-148	<a href="http://www.euro.who.int/document/aiq/5_7dichloromethane.pdf">http://www.euro.who.int/document/aiq/5_7dichloromethane.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	RIVM have adopted WHO approach. See above	RIVM have adopted WHO approach. See above	RIVM have adopted WHO approach. See above	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Chronic inh. To determine NOAEL	To determine a NOAEL for toxicity and carcinogenicity exposure concentrations of 0, 50, 200 and 500ppm selected. Sprague Dawley Rats exposed for 6hrs/day and 5 days/week for 2 years. NOAEL of 50 ppm identified and used to determine MRL	Liver: Hepatocellular cytoplasmic vacuolisation consistent with fatty changes and multinucleated hepatocytes	Nitsche KD, Burek JD, Bell TJ, et al 1988a. Methylene Chloride: A 2-year inhalation toxicity and oncogenicity study in rats. Fundam Appl Toxic 11:60-67.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp14-a.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp14-a.pdf</a>
ATSDR 2		Acute symptoms associated with oxygen deprivation as a result of carboxyhaemoglobin accumulation	No Info		<a href="http://www.atsdr.cdc.gov/MHMI/mmg14.pdf">http://www.atsdr.cdc.gov/MHMI/mmg14.pdf</a>

ID oral					

Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	mouse/B6C3F1	B6C3F1 mice received 0, 60, 125, 185, or 250 (mg/kg)/day of dichloromethane in drinking water. Treatment groups consisted of 50 female mice and 200, 100, 100, and 125 male mice (low to high dose). One hundred females and 125 males served as controls.	Male mice had an increased incidence of combined neoplastic nodules and hepatocellular carcinoma (24/125, 51/200, 30/100, 31/99, 35/125). The increase was not dose-related, but the pair wise comparisons for the two mid- dose groups were reported to be statistically significant (U.S. EPA, 1985a). The hepatocellular carcinoma incidence alone for male mice (which was about 55 to 65% of the total) was not significantly elevated.	NCA (National Coffee Association). 1983. Twenty-four month oncogenicity study of methylene chloride in mice. Final Report. Prepared by Hazleton Laboratories, America, Inc., Vienna, VA.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ic5VI3:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ic5VI3:1</a>
Toxicology Data Network (Toxnet)	See IRIS data	See IRIS data	See IRIS data		<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ic5VI3:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ic5VI3:1</a>

Dichloromethane		CAS Number:	75-09-2	Assessor A:	Nick Brown, Grontmij	Assessor B:	Catherine Helm, WD Environmental	Final Review:	Panel/SF
		Date:	26/05/2009	Date:	01-Jun-09	Date:	28/08/2009		
ID inhal		Recommended IDInhal	Units		Justification				
		N/A	ug.kg-1.d-1		<p>Human studies are considered generally inadequate to demonstrate whether or not DCM is carcinogenic, however, carcinogenicity has been demonstrated in mice and to a lesser extent in female rats. IRIS provides the carcinogenic Classification —B2; probable human carcinogen. IARC classified dichloromethane as possibly carcinogenic to humans (Group 2B), based on inadequate evidence for the carcinogenicity of dichloromethane in humans and sufficient evidence for the carcinogenicity of dichloromethane in experimental animals. Health Canada classified dichloromethane as "probably carcinogenic to humans" (Group II) and has generated PBK modified TD05 values (5% incidence of tumours). IRIS has also quantified carcinogenic risk by predicting concentrations equivalent to increased cancer risk of E-5. In relation to the tendency for tumor development in mice through exposure to DCM by inhalation, TERA comment that; "there are clear species differences in the putatively carcinogenic pathway of metabolism of dichloromethane which are consistent with the hypothesis that humans are likely to be less sensitive than some species of experimental animals in this regard". RIVM determined that dichloromethane is not considered to be genotoxic to humans, and therefore, derived risk values based on a threshold approach. Threshold based HCVs are also provided by ATSDR and WHO.</p> <p>In view of the uncertainty remaining in relation to the actual carcinogenicity of DCM to humans and uncertainty relating to the methods of quantification of non-threshold risk, particularly in view of the guidance provided within SR2, the selection of conservative TDIs is considered more appropriate at this stage than the derivation Index Doses.</p>				

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>		27/05/2009	Yes		TD05s	2238	mg/m3		Not appropriate to derive a clear value from a TD05. See below for TERA conversion of TD05 to 1:100,000 increased cancer risk	5% increase in tumor incidence (PBK modified TD05)
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		02/04/2009	Yes		Predicted concentration equivalent to carcinogenic risk of E-5	20	ug/m3		5.714	Extrapolation Method — Linearized multistage procedure, extra risk
TOXNET 2	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>		02/04/2009	Yes		Predicted concentration equivalent to carcinogenic risk of E-5	0.44	mg/m3		126	Conversion of Health Canada TD05 to 1:100,000 increased cancer risk by TERA

## Dichloromethane

ID inhal					
Organisation	Study type	Description	Response	Reference	Web link
Health Canada Toxicological Values	Mice Bioassay (NTP 1996)	Multi stage modelling of the incidence of cancer undertaken using data from NTP study (NTP 1996). Clear evidence of increased incidence of lung tumors in female mice identified at 13,880mg/m3.	Pulmonary adenomas and carcinomas	NTP (National Toxicology Program). 1986. Toxicology and carcinogenesis studies of dichloromethane (methylene chloride) (CAS No. 75-09-2) in F344/N rats and B6C3F1 mice (inhalation studies). NTP-TRS-306.	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/dichloromethane/">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/dichloromethane/</a>
USEPA Integrated Risk Information System (IRIS)	F344/N rats and B6C3F1 mice	Groups of 50 each male and female rats and mice were exposed to dichloromethane by inhalation, 6 hours/day, 5 days/week for 2 years . Exposure concentrations were 0, 1000, 2000, or 4000 ppm for rats and 0, 2000, or 4000 ppm for mice. Increased occurrence of cancer in mice and female rats was demonstrated.	Mammary adenomas, fibroadenomas and mononuclear cell leukaemia in female rats. Hepatocellular adenomas and carcinomas and alveolar bronchiolar adenomas and acinaromas in mice	NTP (National Toxicology Program). 1986. Toxicology and carcinogenesis studies of dichloromethane (methylene chloride) (CAS No. 75-09-2) in F344/N rats and B6C3F1 mice (inhalation studies). NTP-TRS-306.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ic5VI3:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~ic5VI3:1</a>
TOXNET 2	See Health Canada	See Health Canada	See Health Canada		<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~9nJJZL:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~9nJJZL:1</a>

Dichloromethane	CAS 75-09-2	Assessor A:	Nick Brown Grontmij	Assessor B	Catherine Helm WD Environmental	Final Review	Panel/SF
		Date	29/05/2009	Date	01/06/2009	Date	28/08/2009

Organisation	Date	Media	Value	Units	Description	Reference	Web link
International Programme on Chemical Safety (IPCS)	14/04/2009	Low in food & water	0				<a href="http://www.who.int/ipcs/en">www.who.int/ipcs/en</a>
Joint Expert Committee on Food Additives (JECFA)	14/04/2009	As per WHO Guidelines for DWQ	As per WHO Guidelines for DWQ	As per WHO Guidelines for DWQ	As per WHO Guidelines for DWQ	As per WHO Guidelines for DWQ	As per WHO Guidelines for DWQ
WHO Guidelines for Drinking Water Quality	14/04/2009	Food and drinking water	0	NA	Estimated uptake from food and drinking water expected to be insignificant	Dichloromethane in Drinking Water. Background to the Development of WHO Guidelines for Drinking Water Quality. WHO 2003 (First Published 1996)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Food and drinking water	0	ug/kg-bw/day	Intake via food and water in the Netherlands is assumed to be negligible	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
Health Canada Toxicological Values	14/04/2009	Food types	19 - 95 (concentration in specific food types)	ug/kg	Data on levels of dichloromethane in foods in Canada are very limited. However DCM concentrations monitored by the Total Diet Program of the U.S. Food and Drug Administration . Levels in ready-to-eat cereals and butter were the highest (95 and 84 ug/kg, respectively), followed by cheese (45 ug/kg), margarine (27 ug/kg), processed foods (34 ug/kg), and peanut butter (19 ug/kg).	Heikes and Hopper, 1986; Heikes, 1987a, 1987b; Draft, 1988	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/dichloromethane/dichloromethane_2-eng.php#a22">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/dichloromethane/dichloromethane_2-eng.php#a22</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Drinking water	<1	ppm	Concentrations of DCM recorded at detectable but low concentrations in drinking water in several US cities in the 1970s. No info from later studies provided	Toxicological Profile for Methylene Chloride. ATSDR, September 2000	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp14-c5.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp14-c5.pdf</a>
		Bottled drinking water	0.059	ppb	DCM detected in bottled water in 2.2% of samples. (Page et al. 1993)		
Toxicological Data Network (TOXNET)	14/04/2009	Various food types	<98	ppb	Low concentrations of DCM recorded in specific food types	Heikes DL, Hopper ML; J Assoc Off Anal Chem 69: 990-8 (1986) (2) Heikes DL; J Assoc Off Anal Chem 70: 215-26 (1987)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~VTz5nQ:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~VTz5nQ:1</a>

Dichloromethane	CAS 75-09-2	Assessor A:	Nick Brown Grontmij	Assessor B	Catherine Helm WD Environmental	Final Review		Panel/SF	
		Date	29/05/2009	Date	01/06/2009	Date		Date	28/08/2009
<b>MDI</b>		<b>Recommended MDlinhal</b>		<b>Units</b>		<b>Justification:</b> Based on the value provided by RIVM, converted assuming a 70kg adult.			
		350		ug day-1					
Organisation	Date	Media	Value	Units	Description	Reference	Web link		
International Programme on Chemical Safety (IPCS)	14/04/2009	As per WHO AQG for Europe	As per WHO AQG for Europe	As per WHO AQG for Europe	As per WHO AQG for Europe	As per WHO AQG for Europe	As per WHO AQG for Europe		
Joint Expert Committee on Food Additives (JECFA)	14/04/2009	AS per WHO Guidelines for DWQ	AS per WHO Guidelines for DWQ	AS per WHO Guidelines for	AS per WHO Guidelines for DWQ	AS per WHO Guidelines for DWQ	AS per WHO Guidelines for DWQ		
WHO Guidelines for Drinking Water Quality	14/04/2009	Urban Air	33-307	ug/day	Estimated uptake from urban air	Dichloromethane in Drinking Water. Background to the Development of WHO Guidelines for Drinking Water Quality. WHO 2003 (First Published 1996)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/dichloromethane.pdf</a>		
WHO Air Quality Guidelines for Europe	14/04/2009	Indoor Air	16.3	ug/m3	National Pilot Study in Canadian Homes (757 homes)	WHO Regional Office for Europe, Copenhagen, Denmark. 2000, Air Quality Guidelines 2nd Edition	<a href="http://www.euro.who.int/document/aig/5_7dichloromethane.pdf">http://www.euro.who.int/document/aig/5_7dichloromethane.pdf</a>		
		Indoor Air	9.1 - 26.9	ug/m3	Small survey in Toronto. (Chan et al. 1990)				
		Air	0.5 - 9.9	ug/m3	22 locations across Canada in 1991 - 1992 (Dann T, 1993)				
		Air	0 - 570	ug/m3	20 cities across the US (Macalister R. et. Al. 1989)				
		Air	1.8-3.1	ug/m3	Annual mean concentration at three sites within the San Francisco Bay Area over a four year period (Shiyaki et al 1984)				
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Air	5	ug/kg-bw/day	Estimated intake for the Netherlands is based on a Canadian study. Intake is expected to be primarily through inhalation indoors. Sug/kg-bw/day is equivalent to 350ug/day for a 70kg adult	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>		
Health Canada Toxicological Values	14/04/2009	Air	0.5 - 9.9	ug/m3	22 locations across Canada in 1991 - 1992	Dann T, 1993	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/dichloromethane/dichloromethane_2-eng.php#a22">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/dichloromethane/dichloromethane_2-eng.php#a22</a>		
		Ambient Air	2.6	ug/m3	average from 17 urban sites across Canada	Environment Canada, 1991			
		Indoor Air	16.3	ug/m3	National Pilot Study in Canadian Homes (757 homes)	Otson et al.1992			
		Indoor Air	9.1 - 26.9	ug/m3	Small survey in Toronto.	Chan et al. 1990			
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Background concentration in air	0.17	ug/m3	No detail of study. (Singh et al. 1982)	Toxicological Profile for Methylene Chloride. ATSDR, September 2000	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp14-c5.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp14-c5.pdf</a>		
		Outdoor air	0.61 - 1.62	ug/m3	Range of concentrations recorded in Arizona. Maximum recorded in urban Phoenix (Zielinski et al. 1998)				
					Concentrations likely to be higher in indoor air				
Toxicological Data Network (TOXNET)	14/04/2009	Outdoor air	0.5	ug/m3	A mean concentration detected in 2966 air samples collected from 78 sites in populated areas of the US	Kelly TJ et al; Environ Sci Technol 28: 378A-387A (1994)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/temp/~VTz5nQ:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/temp/~VTz5nQ:1</a>		
		Indoor Air	170	ug/m3	Dichloromethane was detected in 41 of 101 indoor air samples collected from several dwellings in several countries between 1978 and 1990. AVG max concentration of 170ug/m3	Brown SK et al; Indoor Air 4:123-34 (1994)			
			2.6 - 119.7	ug/m3	DCM recorded in a new federal office building in Portland, Oregon between August 1987 and October 1988 at concns ranging from 2.6 to 119.7 ug/cu m	Hodgson AT et al; Air Waste Manag Assoc 41: 1461-68 (1991)			

Substance:		Dichloromethane		CAS Number:		75-09-2		Assessor A:		Claire Potter		Assessor B:		Catherine Heim WD		Final Review:		Panel/SF												
Chemical Formula:		CH2CL2		Phase at Ambient Temperature:		Liquid		Date:		01-Apr-09		Date:		01/06/2009		Date:		28/08/2009												
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H		
							HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCK, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000		
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	84.93	n/a	Median value from consistent (high) range of literature values	Average	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	3.00E+02	25	Median = 264 Min = 241 (-14%) Max = 300 (+14%) therefore not a consistent range  Adopted value is that from the newest source (Lide 2008), which is the max value in range	Geomean	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	2.01E+04	10	newest value in inconsistent range of values provided in Mackay 2006 (also median value of five values in range obtained Mackay and IUPAC-NIST)	Geomean	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
Chemical Boiling Point (ambient pressure)	K	n/a	3.13E+02	n/a	Median value from consistent (high) range of literature values	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Chemical Melting Point (ambient pressure)	K	n/a	1.78E+02	n/a	Median value from consistent (high) range of literature values	Average	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Log Octanol - Water Coefficient	Dimensionless	n/a	1.28	n/a	Median value from consistent (medium) range of literature values	Average	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	7.14E+01	n/a	Single literature value available	Average	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	27878.8315	2.79E+04	Normal Chemical Boiling Point	Calculated Value (below minimum in range (low consistency) of literature values)	Average	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Chemical Critical Point temperature (ambient pressure)	K	506.4036603	5.06E+02	n/a	Calculated Value (below minimum in range (low consistency) of literature values)	Average	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Critical Pressure	atm	58.29705069	5.83E+01	Not stated	Calculated Value (below minimum in range (low consistency) of literature values)	Average	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	5.636E-02	10	Estimated from parameters above using Clapyron relationship or direct calculation
Vapour pressure at ambient soil temperature	Pa	31370.90089	10	Estimated from parameters above using Grain-Watson method
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	9.97E-06	10	Estimated from parameters above using Wilkie-Lee method
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	7.91E-10	10	Estimated from parameters above using Hayduk and Laudie method
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	1.14	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Diethyl Phthalate	CAS Number:	84-66-22	Assessor A:	Mathew Rouge	Assessor B:	Gareth Wills	Final Review:	Panel/SF
			Date:	March 09	Halcrow	Date:	April 09	PB
							Date:	26/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	Yes	TDloral applied to oral and dermal routes. Not classifiable as a human carcinogen. Not classifiable as a human carcinogen. Insufficient data with sufficient detail on derivation to derive inhalation TDI. Use route-to-route extrapolation from oral route.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	200	ug.kg-1.d-1	Most conservative value chosen (RIVM and EC SCF), based on longest term study (Brown et al 1978). RfD from IRIS has low confidence, although is taken from same study (Brown et al, 1978).

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	2003	Mar-09	TDI	5000	ug/kg/bw/day	5000	Not provided	NOAEL	1600	mg/kg bw/day	300	3 for incompleteness of database, 10 each for intra and interspecies variation
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	TDI (Provisional). It was adopted from the European Communities temporary limit value of 0.2 mg/kg/day	200	ug/kg/bw/day	200	Not provided	NOAEL	100	mg/kg bw/day	500	intra and interspecies extrapolation and a poor database
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	1995	Mar-09	Database not adequate for determination of a chronic MRL	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	1995	Mar-09	acute oral MRL	7	mg/kg bw/d	7,000	Not provided	LOAEL	2000	mg/kg bw/d	300	3 for conversion of minimal LOAEL to NOAEL, 10 for interspecies variability, 10 for protection of sensitive humans
	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	1995	Mar-09	intermediate duration oral MRL	6	mg/kg bw/d	6,000	Not provided	LOAEL	1753	mg/kg bw/d	300	3 for conversion of minimal LOAEL to NOAEL, 10 for interspecies variability, 10 for inter individual variation
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1993	Mar-09	RfD	8.00E-01	mg/kg/d	800	Study - Medium, Database - Low, RfD - Low	NOAEL:1% of diet (750 mg/kg bw/day)	800	mg/kg bw/day	1000	10 extrapolation from subchronic to chronic, 10 for interspecies variation and an additional 10-fold factor to protect sensitive human subpopulation
EC Scientific Committee for Food	<a href="http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/82phthal.htm">http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/82phthal.htm</a>	1996	Mar-09	Oral TDI	0.2	mg/kg bw/d	200	Not Provided	Not Provided	Not Provided	Not Provided	Not Provided	Not Provided

## Diethyl Phthalate

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
IPCS concise International Chemical Assessment Documents (CICADs)	Mice, dermal study	Diethylphthalate at 500, 1600 and 5600 mg/kg bw/day administered percutaneously to pregnant ICR mice from day 0 to day 17 of gestation	Reproductive toxicity	Tanaka C et al, (1987) A teratological evaluation following dermal application of diethylphthalate to pregnant mice	<a href="http://inchem.org/documents/cicads/cicads/cicad52.htm">http://inchem.org/documents/cicads/cicads/cicad52.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Rat, Subchronic Oral Feeding Study. Brown et al, 1978	Groups of CD rats (15/sex) were fed diets containing 0, 0.2, 1.0, or 5.0% DEP for 16 weeks	liver and testes	Brown, D., K.R. Butterworth, I.F. Gaunt, P. Grasso and S.D. Gangolli. 1978. Short-term oral toxicity study of diethyl phthalate in the rat. Food Cosmet. Toxicol. 16: 415-422	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp73.html">http://www.atsdr.cdc.gov/toxprofiles/tp73.html</a>
	acute rat study	2 day study, rats received 2,000 mg/kg bw/d DEP for 2 days by gavage	Leydig cell ultra structural changes	Jones et al 1993	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp73.html">http://www.atsdr.cdc.gov/toxprofiles/tp73.html</a>
	male rat study		peroxisomal proliferation, slightly elevated liver weight, changes in hepatic enzyme activities	Moody and Reddy 1978	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp73.html">http://www.atsdr.cdc.gov/toxprofiles/tp73.html</a>
USEPA Integrated Risk Information System (IRIS)	Rat, Subchronic Oral Feeding Study. Brown et al, 1978	Groups of CD rats (15/sex) were fed diets containing 0, 0.2, 1.0, or 5.0% DEP for 16 weeks	Decreased growth rate, food consumption and altered organ weights	Brown, D., K.R. Butterworth, I.F. Gaunt, P. Grasso and S.D. Gangolli. 1978. Short-term oral toxicity study of diethyl phthalate in the rat. Food Cosmet. Toxicol. 16: 415-422	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>
EC Scientific Committee for Food	Not Provided	Not Provided	Not Provided	Not Provided	<a href="http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/82phthal.htm">http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/82phthal.htm</a>

Diethyl Phthalate	CAS Number:	84-66-22	Assessor A:	Mathew Rouge	Assessor B:	Gareth Wills	Final Review:	Panel/SF
			Date:	March 09	Halcrow	Date:	April 09	PB
						Date:	26/08/2009	

TDI inhal	Recommended TDI <sub>inhal</sub>	Units	Justification
	N/A	ug/kg bw/d	Insufficient data with sufficient detail on derivation to derive inhalation TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	2007	Mar-09	Workplace Exposure Limit	5	mg/m3	1428.6 ug/kg bw/d	Not provided	Not provided	Not provided	Not provided	Not provided	Not provided
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2000	Mar-09	TCA not derived due to lack of appropriate data; and moreover, that inhalation exposure is considered not relevant due to low volatility	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	1995	Mar-09	No chronic MRL derived because the only available inhalation study was limited	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>	2008	Mar-09	RfC (RS-ESL)	0.005	mg/m3	1.429 ug/kg bw/d	Not provided	no information on provenance	Not provided	Not provided	Not provided	Not provided

ID oral	Recommended ID <sub>oral</sub>	Units	Justification
	N/A		not classifiable as a human carcinogen

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1993	Mar-09	No quantifiable estimate available. Classification - D; not classifiable as a human carcinogen	n/a	n/a	n/a	n/a	n/a	n/a	n/a

ID inhal	Recommended ID <sub>inhal</sub>	Units	Justification
	N/A		not classifiable as a human carcinogen

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	1993	Mar-09	No quantifiable estimate available. Classification - D; not classifiable as a human carcinogen	n/a	n/a	n/a	n/a	n/a	n/a

## Diethyl Phthalate

## TDI inhal

Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Health and Safety Executive (HSE)	Not provided	8 hour long term workplace exposure limit	Not provided	Not provided	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	n/a	n/a	n/a	n/a	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	n/a	n/a	n/a	n/a	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp73.html">http://www.atsdr.cdc.gov/toxprofiles/tp73.html</a>
Texas Commission on Environmental Quality	Not provided	Not provided	Not provided	Not provided	<a href="http://www.tceq.state.tx.us/remediation/rrr.html">http://www.tceq.state.tx.us/remediation/rrr.html</a>

## ID oral

Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

## ID inhal

Organisation	Study type	Description	Response	Reference	Web link
USEPA Integrated Risk Information System (IRIS)	n/a	n/a	n/a	n/a	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>

Diethylphthalate	CAS 84-66-2	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
		Date:	08/04/2009	Date:	15/04/2009	Date:	26/08/2009

MDI	Recommended MDIoral	Units	Justification: relatively new (Ursel et al. 2007) study, mean exposure to 8 phthalates in 5 consumer groups.
	80.5	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
IPCS Concise International Chemical Assessment Documents (CICADs)	2000	Surface Water	1	ug day-1	In a compilation of concentrations (1984–1997) of diethyl phthalate in North American and western European surface waters (USA, Canada, United Kingdom, Germany, Netherlands, Sweden), geometric mean concentrations ranged from about 0.01 to 0.5 µg/litre (Staples et al., 2000). Using the highest mean the average daily intake through water consumption would be 1 ug day (Using the CLEA calculation of 2 litres per day intake)	Staples CA, Parkerton TF, Peterson DR (2000) A risk assessment of selected phthalate esters in North American and Western European surface waters. <i>Chemosphere</i> , 40:885–891	<a href="http://incchem.org/documents/cicads/cicads/cicad52.htm">http://incchem.org/documents/cicads/cicads/cicad52.htm</a>
	2001	Food	0.35	ug day-1	In a duplicate-portion study, Tsumura et al. (2001) estimated daily intake of 11 phthalate esters, including diethyl phthalate and di(2-ethylhexyl) adipate, in 1-week total diet samples provided in hospitals. Portions of meals of breakfast, lunch, and supper were obtained from three hospitals located in three areas in Japan in October or December 1999, for a period of 7 days. Recovery of the spiked samples and quality assurance of analysis were performed at three laboratories. Daily intakes of diethyl phthalate were 0.07–1.41 µg/person (samples in which diethyl phthalate was not detected were assumed to contain diethyl phthalate at 50% of the limit of detection, which was 0.1, 0.2, and 0.5 ng/g for the three participating laboratories after subtraction of the blank value). Average daily intakes in the three hospitals were estimated to be 0.10, 0.28, and 0.67 µg (overall average 0.35 µg) per day per person, respectively	Tsumura Y, Ishimitsu S, Saito I, Sakai H, Kobayashi Y, Tonogai Y (2001) Eleven phthalate esters and di(2-ethylhexyl)adipate in one-week duplicate diet samples obtained from hospitals and their estimates of daily intake. <i>Food Additives and Contaminants</i> , 18(5):449–460	<a href="http://incchem.org/documents/cicads/cicads/cicad52.htm">http://incchem.org/documents/cicads/cicads/cicad52.htm</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	1976	Drinking Water	0.2	ug day-1	Diethyl phthalate was found in the finished drinking water of 6 of 10 U.S. cities at concentrations of 0.01 µg/L (Seattle, Washington; Philadelphia, Pennsylvania; New York, New York) Based on this concentration the daily intake is calculated to be 0.2 ug day, assuming 2 litres intake a day.	Keith et al 1976. Identification of organic compounds in drinking water from thirteen US cities. In: Keith LH, ed. Identification and analysis of organic pollutants in water. Ann Arbor, MI: Ann Arbor Press, 329-373	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp73.html">http://www.atsdr.cdc.gov/toxprofiles/tp73.html</a>
	1991	Food	4000	ug day-1	Estimated to be 4mg day based on a consumption of 1kg of food wrapped in cellulose acetate containing diethyl phthalate at a concentration of 4 mg/kg (Karmin and Mayor, 1991)	Kamrin MA, Mayor GH. 1991. Diethyl Phthalate - a perspective. <i>J Clin Pharmacol</i> 31(5):484-489	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp73.html">http://www.atsdr.cdc.gov/toxprofiles/tp73.html</a>
Entrez PubMed	2003	Total Intake	1547	ug day-1	A study on the German population found that the 95th percentile of the population studied had an intake of diethylphthalate of 22.1 ug/kg bw/day. The study used excreted metabolites in urine to determine the intake concentration of the individual.	Koch HM, Drexler H, Angerer J, (2003) An estimation of the daily intake of di(2-ethylhexyl)phthalate (DEHP) and other phthalates in the general population, <i>International Journal Hyg Environmental Health</i> . 2003 Mar;206(2):77-83	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>
Other	2007	Total Intake	80.5	ug day-1	Daily internal exposure to eight phthalates (in µg/kg bodyweight day) in 5 consumer groups, mean and maximal exposure – estimations based on ambient monitoring and scenario calculations for uptake of food, air, water, consumer products, household dust, leaching from toys, etc. Adult mean daily intake of diethyl phthalate was 1.15 ug/kg bw/day with the maximum being 50.94. Using the 1.15 value a daily intake has been calculated as 80.5 ug day	Ursel Heudorf, Volker Mersch-Sundermann and Jürgen Angerer (2007), Phthalates: Toxicology and exposure <i>International Journal of Hygiene and Environmental Health</i> Volume 210, Issue 5, 31 October 2007, Pages 623-634, Children's Environment in Central Europe - Threats and Chances - Results of an International Workshop held on November 21-24, 2006 in Osnabrück	<a href="http://www.sciencedirect.com/science?_ob=ArticleURL&amp;_udi=B7GVY-4PPWMN9-3&amp;user=10&amp;rdoc=1&amp;fmt=&amp;orig=search&amp;sort=d&amp;docanchor=&amp;view=c&amp;acct=C000050221&amp;version=1&amp;urlVersion=0&amp;userid=10&amp;md5=24db0bb7c2fd9a3feb87b30f3af5d14d">http://www.sciencedirect.com/science?_ob=ArticleURL&amp;_udi=B7GVY-4PPWMN9-3&amp;user=10&amp;rdoc=1&amp;fmt=&amp;orig=search&amp;sort=d&amp;docanchor=&amp;view=c&amp;acct=C000050221&amp;version=1&amp;urlVersion=0&amp;userid=10&amp;md5=24db0bb7c2fd9a3feb87b30f3af5d14d</a>
MAFF	1996	Food	100 - 800	ug day-1	MAFF Food Surveillance Information Sheet 82. Total Diet Study identified between 0.1 to 0.8 mg/day exposure to total phthalates within food		<a href="http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/82phthal.htm">http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/82phthal.htm</a>

Diethylphthalate		CAS 84-66-2	Assessor A:	Gareth Wills	Assessor B:	Mat Rouge	Final Review:	Panel/SF
			Date:	08/04/2009	Date:	15/04/2009	Date:	26/08/2009
<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Although value is based upon indoor air study in Japan (Takamitsu Otake, Jun Yoshinaga and Yukio Yanagisawa), alternative values are based on monitoring at known DEP source zones, and therefore overly estimate exposure. Converted from 0.1µg/m <sup>3</sup> assuming 20m <sup>3</sup> /day air inhaled.			
			2	ug day-1				
Organisation	Date	Media	Value	Units	Description	Reference	Web link	
IPCS Concise International Chemical Assessment Documents (CICADs)	1987	Indoor Air	40.6	ug day-1	Diethyl phthalate has been measured in the indoor air of a telephone switching office and in outdoor air in Newark, USA, at concentrations ranging from 1.60 to 2.03 µg/m <sup>3</sup> and from 0.40 to 0.52 µg/m <sup>3</sup> , respectively, during a 43-day sampling period (Shields & Weschler, 1987) - which taking the highest recorded value converts to a daily intake of 40.6 ug day using the CLEA intake value of 20 m <sup>3</sup> per day	Shields HC, Weschler CJ (1987) Analysis of ambient concentrations of organic vapors with a passive sampler. <i>Journal of the Air Pollution Control Association</i> , 37(9):1039-1045	<a href="http://inchem.org/documents/cicads/cicads/cicad52.htm">http://inchem.org/documents/cicads/cicads/cicad52.htm</a>	
Toxicological Data Network (TOXNET)	1984	Ambient Air	0.002	ug day-1	Diethyl phthalate was detected in the atmosphere over Barrow, AK at concns of 0.1 ng/cu m - which converts to 0.002 ug day using the CLEA intake value of 20 m <sup>3</sup> per day	Giam CS et al; in Handbook of Environmental Chemistry; Anthropogenic Substances. Berlin, Germany: Springer-Verlag pp. 67-142 (1984)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	
Other	24-Mar-04	Indoor Air	0.1	ug/m <sup>3</sup> (equates to 2 ug/d, assuming 20m <sup>3</sup> air inhaled/d)	Phthalate esters and phosphate esters in samples of indoor air from 27 houses in the Tokyo Metropolitan area were quantified using gas chromatograph/mass spectrometer and gas chromatograph/flame photometric detector after adsorption on to charcoal and solvent extraction. The median concentrations of diethyl phthalate, dibutyl phthalate (DBP), butylbenzyl phthalate, dicyclohexyl phthalate and diethylhexyl phthalate were 0.10, 0.39, 0.01, 0.07 and 0.11 µg/m <sup>3</sup> , respectively.	Takamitsu Otake, Jun Yoshinaga and Yukio Yanagisawa. <i>Journal of Exposure Analysis and Environmental Epidemiology</i> (2004) <b>14</b> , 524-528. doi:10.1038/sj.jea.7500352 Published online 24 March 2004	<a href="http://www.nature.com/jes/journal/v14/n7/full/7500352a.html">http://www.nature.com/jes/journal/v14/n7/full/7500352a.html</a>	



<b>Di methyl phthalate</b>	<b>CAS Number:</b>	<b>131-11-3</b>	<b>Assessor A:</b>	Barry Mitcheson, Enviros	<b>Assessor B:</b>	Alison Pugh, Hyder	<b>Final review:</b>	Panel/SF
			<b>Date</b>	05/05/2009	<b>Date</b>	06/05/2009	<b>Date</b>	08/09/2009

	Oral	Dermal	Inhalation	Justification
Apply TDloral to exposure routes?	No	No	No	No strong evidence to be a human carcinogen - Insufficient data to derive TDI
Apply IDoral to exposure routes?	No	No	No	
Apply TDlinh to exposure routes?	No	No	No	No strong evidence to be a human carcinogen - Insufficient data to derive TDI
Apply IDinh to exposure routes?	No	No	No	

<b>TDI oral</b>	<b>Recommended TDI oral</b>	<b>CLEA Units</b>	<b>Justification</b>
	n/a	ug.kg-1.d-1	No suitable study identified. Consideration given to use of DEP as surrogate, as set out by RIVM in report on dust exposure but toxic mechanism of DMP not known, consideration also given to group restriction on all phthalates. Careful consideration should be given to potential additive effects of different phthalates when setting HCVs.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	Friday 5 August 2005 (One site date not given)	31/03/2009											
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	29/4/8 (uploaded infant milk formula file from July 2006)	06/04/2009	TDI	0.05	mg/kgbw/day	50		The Committee was aware that new evidence on the reproductive effects of phthalates has been published since this TDI was set.			100	SCF not details given	NOAEL
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	1999	07/04/2009	TDI tabulated	0.05	mg/kgbw/day	50							
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	copyright 2005	19/04/2009						LD50	8200	mg/kg bw			

## Di methyl phthalate

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
<b>Food Standards Agency (FSA)</b>	Reference to Endocrine disruptors on infomaiton page. The site states that the European Food Safety Authority reviews all the scientific data in order to set a tolerable daily intake. This is an estimate of the amount of a substance in food or drinking water that can be consumed daily by people over a lifetime without any appreciable risk to health.			<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
<b>Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)</b>	Reference made in Jul 1996 STATEMENT ON PHTHALATES IN INFANT FORMULAE to Tolerable Daily Intakes (TDIs) set by the EC Scientific Committee for Food for a group restriction of 0.05mg/kg bw/day. Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. These exceed by 2-3 fold the temporary "group restriction" of 0.05 mg/kg bodyweight/day set by the SCF for those phthalates for which further toxicity testing is required. The Committee notes that TDIs are derived from doses which produce no effect in animal studies		Jul 1996 STATEMENT ON PHTHALATES IN INFANT FORMULAE Variability and Uncertainty in Toxicology of Chemicals in Food, Consumer Products and the Environment March 2007 looks at phthalate esters as endocrine modulators affecting testes and exposure of rats during pregnancy to high levels of certain phthalate esters is able to induce in the male offspring a collection of disorders that is remarkably similar to Testicular Dysgenesis Syndrome in humans and in foetal life a substantial reduction in anogenital distances. also in TOX/2003/09 COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD, CONSUMER PRODUCTS AND THE ENVIRONMENT ADVERSE TRENDS IN DEVELOPMENT OF THE MALE REPRODUCTIVE SYSTEM - POTENTIAL CHEMICAL CAUSES 2003 and annual report 2006)	<a href="http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf">http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf</a> also in <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> referring to SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a> (Other sites with no dose data <a href="http://cot.food.gov.uk/pdfs/vutreportmarch2007.pdf">http://cot.food.gov.uk/pdfs/vutreportmarch2007.pdf</a> , <a href="http://cot.food.gov.uk/pdfs/2003-09endocrine.PDF">http://cot.food.gov.uk/pdfs/2003-09endocrine.PDF</a> , <a href="http://cot.food.gov.uk/pdfs/cotsection06.pdf">http://cot.food.gov.uk/pdfs/cotsection06.pdf</a> )
<b>Scientific Committee on Food (SCF) pre 2002</b>	Available limited oral rat chronic toxicity/carcinogenicity, oral teratogenicity studies in rats and mice, Ames test. . Needed : gene mutation and chromosome aberration in mammalian cells in vitro and migration data in the first instance		Compilation of the Evaluations of the scientific committee on food on certain monomers and additives used in the manufacture of plastics materials intended to come into contact with food Stuffs Until 21 March 1997 SCF 1999	<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf</a>
<b>WHO Guidelines for drinking water Quality</b>	mg of toxicant per kg bw required to kill 50% of large population of test animals. Used in repellent. In table 5 which is for active ingredients unlikely to present active hazard in normal use		The WHO recommended classification of pesticides by hazard and guidelines to classification : 2004.	<a href="http://www.who.int/ipcs/publications/pesticides_hazard_rev_3.pdf">http://www.who.int/ipcs/publications/pesticides_hazard_rev_3.pdf</a>

Di methyl phthalate		CAS Number:	131-11-3	Assessor A:	Barry Mitcheson, Enviros	Assessor B:	Alison Pugh, Hyder	Final review:	Panel/SF						
				Date	05/05/2009	Date	06/05/2009	Date	08/09/2009						
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009												
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	1989	20/04/2009						NOAEL	1% DMP = 0.8	g/kg/day				rats
		1989	20/04/2009						NOAEL	5% DMP = 3.6	g/kg/day				rats
TDI inhal				Recommended TDI inhal	n/a	CLEA Units	ug.kg-1.d-1	Justification							
				No suitable study identified. Consideration given to use of DEP as surrogate set out by RIVM in report on dust exposure but toxic mechanism of DMP not known, consideration also given to group restriction on all phthalates. Careful consideration should be given to potential additive effects of different phthalates when setting HCVs.											
Organisation		Last Updated		Health criteria type	Value		Units	Confidence rating	Basis	Value	Units	UF	UF description	Study type	
Drinking Water Inspectorate (DWI)	<a href="http://www.dwi.gov.uk/">http://www.dwi.gov.uk/</a>	31-Mar-09													
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	Friday 5 August 2005 (One site date not given)	31/03/2009												
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>		06/04/2009	HSC/04/06 Annex C. WEL 5mg/m3 and STEL 10mg/m3. Risk Phrases refer to R60 and R61 (harm fertility and harm the unborn child) and R50 toxic to aquatic organisms											
IPCS INCHEM	<a href="http://inchem.org/">http://inchem.org/</a>		07/04/2009	Occupational health limits 5mg/m3											
Joint FAO/WHO Meeting on Pesticide Residues (JMPR)	<a href="http://www.who.int/ipcs/food/impr/en/">http://www.who.int/ipcs/food/impr/en/</a>		08/04/2009												
JMPR 2	<a href="http://inchem.org/pages/impr.html">http://inchem.org/pages/impr.html</a>		08/04/2009												
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009												
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	1980 (abstract only)	20/04/2009	Maximum Allowable concentration (MAC)	0.3		mg/m3								
		2008	20/04/2009	OSHA standards - permissible exposure limit	5		mg/m3								
		2005	20/04/2009	NIOSH - recommended exposure limit	5		mg/m3								
		2005	20/04/2009	NIOSH - immediately dangerous to Life or Health	200		mg/m3								

Di methyl phthalate				
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	TDI of dimethyl phthalate (DMP) is unknown as the compound is chemically comparable to diethyl phthalate (DEP), the concentrations of DMP are added to the concentrations of DEP and compared to the TDI of DEP. 200ug/kgbw/day		Re-evaluation of human-toxicological Maximum Permissible Levels. Report no. 711701025,	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Toxicology Data Network (Toxnet)	Maternal toxicity		Developmental Toxicity of Dimethyl phthalate (CAS No. 131-11-3) Administered to CD Rats on Gestational Days 6 Through 15	<a href="http://ntp.niehs.nih.gov/index.cfm?objectid=07305BCA-A86E-545E-0669D64152F6C5BC">http://ntp.niehs.nih.gov/index.cfm?objectid=07305BCA-A86E-545E-0669D64152F6C5BC</a>
	development toxicity		Developmental Toxicity of Dimethyl phthalate (CAS No. 131-11-3) Administered to CD Rats on Gestational Days 6 Through 15	<a href="http://ntp.niehs.nih.gov/index.cfm?objectid=07305BCA-A86E-545E-0669D64152F6C5BC">http://ntp.niehs.nih.gov/index.cfm?objectid=07305BCA-A86E-545E-0669D64152F6C5BC</a>
TDI inhal				
Organisation	Description	Response	Reference	Web link
Drinking Water Inspectorate (DWI)	No dose data identified - searched for plasticiser, phthalate, dicarboxylic. Note that tests for plastic pipes must comply with BS 6920 which includes a flavour and odour test			
Food Standards Agency (FSA)	Not data on inhalation dose. Reference make to endocrine disruptors. Site relates to contact with food			<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
Health and Safety Executive (HSE)				<a href="http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf">http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf</a>
IPCS INCHEM			Di methyl phthalate ICSC 0261	<a href="http://www.inchem.org/documents/icsc/icsc/eics0261.htm">http://www.inchem.org/documents/icsc/icsc/eics0261.htm</a>
Joint FAO/WHO Meeting on Pesticide Residues (JMPR)	reference to phthalates only relate to DMP as solvent for dermal test and DEHP and as interference			
JMPR 2	reference to phthalates only relate to DMP as solvent for dermal test and DEHP and as interference			
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	No assessment of inhalation due to low volatility, but Oral dose for DEP used for dust inhalation in paper.		Re-evaluation of human toxicological maximum permissible levels (Baars 2001)	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Toxicology Data Network (Toxnet)			Toxicology of esters of O-phthalic acid and hygienic standards for them. GIG TR PROF ZABOL; 0 (3). 1980. 28-29	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~ggmhOT:21">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~ggmhOT:21</a>
			Occupational Health Standards - OSHA from HSDB	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~eWqfYa:7">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~eWqfYa:7</a>
			Occupational Health Standards - NOISH from HSDB	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~eWqfYa:7">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~eWqfYa:7</a>
			Occupational Health Standards - NOISH from HSDB	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~eWqfYa:7">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~eWqfYa:7</a>

Di methyl phthalate		CAS Number:	131-11-3	Assessor A:	Barry Mitcheson, Enviros	Assessor B:	Alison Pugh, Hyder	Final review:	Panel/SF
		Date	05/05/2009	Date	06/05/2009	Date	08/09/2009		

ID oral	Recommended ID oral	CLEA Units	Justification
	n/a		Insufficient evidence for classification

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
Drinking Water Inspectorate (DWI)	<a href="http://www.dwi.gov.uk/">http://www.dwi.gov.uk/</a> 31-Mar-09								
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a> Friday 5 August 2005 (On 31-Mar-09)	31/03/2009							
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	07/04/2009							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a> 01/02/1990 (database last commented in 1998)	08/04/2009							

ID inhal	Recommended Id inhal	CLEA Units	Justification
	n/a		Insufficient evidence for classification

Organisation	Last Updated	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a> 06/04/2009								
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	07/04/2009							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a> 01/02/1990 (database last commented in 1998)	08/04/2009							

Di methyl phthalate

ID oral				
Organisation	Description	Response	Reference	Web link
Drinking Water Inspectorate (DWI)	No dose data identified - searched for plasticiser, phthalate, dicarboxylic. Note that tests for plastic pipes must comply with BS 6920 which includes a flavour and odour test			
Food Standards Agency (FSA)	Site refer to endocrine disruptors not to carcinogenicity			<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
Scientific Committee on Food (SCF) pre 2002	Genotoxic and chromosome aberration tests required		Compilation of the Evaluations of the scientific committee on food on certain monomers and additives used in the manufacture of plastics materials intended to come into contact with food Stuffs Until 21 March 1997 SCF 1999	<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Classification — D; not classifiable.  Basis — Pertinent data regarding carcinogenicity was not located in the available literature.			<a href="http://www.epa.gov/ncea/iris/subst/0353.htm">http://www.epa.gov/ncea/iris/subst/0353.htm</a>

ID inhal				
Organisation	Description	Response	Reference	Web link
Health and Safety Executive (HSE)	HSC/04/06 Annex C All three listed. WEL 5mg/m3 and STEL 10mg/m3. Risk Phrases refer to R60 and R61 (harm fertility and harm the unborn child) and R50 Very toxic to aquatic organisms			<a href="http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf">http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf</a>
Scientific Committee on Food (SCF) pre 2002	Genotoxic and chromosome aberration tests required		Compilation of the Evaluations of the scientific committee on food on certain monomers and additives used in the manufacture of plastics materials intended to come into contact with food Stuffs Until 21 March 1997 SCF 1999	<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Classification — D; not classifiable.  Basis — Pertinent data regarding carcinogenicity was not located in the available literature.			<a href="http://www.epa.gov/ncea/iris/subst/0353.htm">http://www.epa.gov/ncea/iris/subst/0353.htm</a>

Substance:		Dimethyl phthalate		CAS Number:		131-11-3		Assessor A:		Alison Pugh, Hyder		Assessor B:		Tim Rolfe, Enviro		Final review:		Panel/SF																
Chemical Formula:		C10H10O4		Phase at Ambient Temperature:		Liquid		Date:		02-Apr-09		Date:		30-Apr-09		Date:		08/09/2009																
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000						
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	
<b>Required Parameters</b>																																		
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	194.18	n/a	High Consensus between sources		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)				
						Average	194.2	194.2	n/a	194.184	194.184	n/a	194.184	194.184	n/a	194.18	194.18	n/a	194.19	194.19	n/a	194.17	194.17	n/a	194.17	194.17	n/a	Insert Values	Insert Values	n/a				
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	1.92E+00	25	Geomean value from Montgomery (as wide range of data)		atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	KPa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	Pa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)				
						Geomean	1.10E-07	1.11E-02	25	Insert Values	Insert Values	25	1.11E-01	0.111	0.111	0.011	0.011	0.218	0.012	0.00978	0.00978	25	n/a	n/a	n/a	1.68E-05	1.70226	4.20E-07	0.0425565	25	Insert Values	25	Insert Values	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	4.00E+03	25	Several references the same - Howard, Lide, Montgomery		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	
						Geomean	4.00E+03	4.00E+03	25	4.00E+00	4000	25	3.97E+03	3.97E+03	25	4.30E+03	4.30E+03	25	4.32E+03	4.32E+03	25	4.32E+03	4.32E+03	25	4.32E+03	4.32E+03	25	Insert Values	Insert Values	25	Insert Values	25		
Chemical Boiling Point (ambient pressure)	K	n/a	5.57E+02	n/a	High Consensus between sources		°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°K	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	
						Average	283.7	556.85	n/a	283.7	556.85	n/a	283.7	556.85	n/a	283.7	556.85	n/a	283.7	556.85	n/a	283.8	556.95	n/a	283.8	556.95	n/a	Insert Values	Insert Values	n/a	Insert Values	n/a		
Chemical Melting Point (ambient pressure)	K	n/a	2.79E+02	n/a	High Consensus between sources		°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	°K	°K	Ref. Temp (C)	°C	°K	Ref. Temp (C)	
						Average	5.5	278.65	n/a	5.5	278.65	n/a	5.5	278.65	n/a	5.5	278.65	n/a	0	273.15	n/a	5.5	278.65	n/a	5.5	278.65	n/a	Insert Values	Insert Values	n/a	Insert Values	n/a		
Log Octanol - Water Coefficient	Dimensionless	n/a	1.61E+00	n/a	Mid Range Value - referenced in Mackay, Montgomery		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	
						Average	1.56	1.56	n/a	Insert Values	Insert Values	n/a	1.61	1.61	n/a	Insert Values	Insert Values	n/a	1.53	1.53	n/a	1.53	1.53	n/a	2	2.00	n/a	Insert Values	Insert Values	n/a	Insert Values	n/a		
Molar Volume (Le Bas method)	cm3 mol <sup>-1</sup>	n/a	2.06E+02	n/a	Single reference		n/a	n/a	n/a	n/a	n/a	n/a	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
						Average	n/a	n/a	n/a	n/a	n/a	n/a	206.4	206.40	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	54873.76665	54874	Normal Chemical Boiling Point	Calculated value chosen - this is similar to range of reported values		n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
						Average	n/a	n/a	n/a	Insert Values	Normal Boiling Point	78.66	78660	Normal Boiling Point	78.66	78660	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
Chemical Critical Point temperature (ambient pressure)	oK	766.1623109	766	n/a	Calculated value chosen - this is similar to range of reported values		n/a	n/a	n/a	°K	°K	Ref. Temp (C)	n/a	n/a	n/a	°C	°K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
						Average	n/a	n/a	n/a	772	772.00	n/a	n/a	n/a	n/a	Insert Values	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
Critical Pressure	atm	27.4849242	27.5	n/a	Calculated value chosen - this is similar to range of reported values		n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
						Average	n/a	n/a	n/a	27.7	27.3377449	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	1.578E-04	10	Estimated from parameters above using Clapyron relationship or direct calculation
Vapour pressure at ambient soil temperature	Pa	0.118109354	10	Estimated from parameters above using Grain-Watson method
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	5.33E-06	10	Estimated from parameters above using Wilkie-Lee method
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	4.23E-10	10	Estimated from parameters above using Hayduk and Laudie method
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	1.85	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Di n butyl phthalate, Di butyl phthalate or DBP	CAS Number:	84-74-2	Assessor A:	Barry Mitcheson, Enviroso	Assessor B:	Alison Pugh, Hyder	Final review:	Panel/SF
	Date	05/05/2009	Date	05/05/2009	Date	26/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDioral to exposure routes?	Yes	Yes	No	No	No strong evidence to be a human carcinogen - TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		No strong evidence to be a human carcinogen - TDlinh based on localised effects where additivity unlikely to be relevant.
Apply IDinh to exposure routes?	No	No	No		

TDI oral				Recommended TDI oral	CLEA Units	Justification				
				10	ug.kg-1.d-1	Value selected by EFSA for localised effects based on most recent rat study(2004), which was not considered by most other references.				
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	Friday 5 August 2005 (One site date not given)	31/03/2009	See Description for information						
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>	29/4/8 (uploaded infant milk formula file from July 2006)	06/04/2009	TDI	0.05 mg/kgbw/day	50	Not given. COT noted new evidence on reproductive effects published after TDIs set. The Committee notes that TDIs are derived from doses which produce no effect in animal studies	100	SCF, no details given	
				TDI Oral	2.5 mg/kg bw/day	2500	Low as study not designed for risk assessment	250 mg/kg bw/day	100	Margin of safety used by COT
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search: 1994 Review of report by MS Technical Experts finalised: 1999 Final report: 2003 (The last full literature survey was carried out in 1994 - targeted searches were carried out subsequently).	07/04/2009	TDI	0.052-0.104 mg/kg bw/day	52 - 104	LOAEL of 52 mg/kg bw based on embryotoxic effects in rats is basis for risk assessment. 80mg/kg bw may be more appropriate - see description	52 mg/kg bw/day	500 - 1000	Includes factor of 5 for uncertainty of LOAEL
European Food Safety Authority (EFSA)	<a href="http://www.efsa.europa.eu/en.html">http://www.efsa.europa.eu/en.html</a>	2005		TDI	0.01 mg/kg bw/day	10	LOAEL from developmental study on rats. Not typo in report referring to 20mg/kg bw/day early on)	2 mg/kg bw/day	200	Effects reversible at all dose levels, especially lowest dose (1.5 to 3 mg/kg bw/day) and also findings of several reproductive studies with longer exposure showing 30 -fold higher NOAELs or LOAELs, uncertainty factor of 200 considered sufficient.

**Di n butyl phthalate, Di butyl phthalate or DBP**

TDI oral					
Food Standards Agency (FSA)		Reference to Endocrine disruptors. States that EFSA reviews all the scientific data to set a TDI. <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> - notes provisional TDI of 50ug/kgbw/day for all phthalate esters in contact with food (excluding diethylphthalate = 500ug/kgbw/day SCF (1996)).	Not stated.	Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>	<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	NOAEL	Reference to a group restriction of 0.05mg/kg bw/day. Dibutylphthalate assessed further. References noted other effects but did not provide effect doses - synergistic /antagonistic effects with TCE and haptachlor, exposure of rats to high levels during pregnancy inducing a disorders in offspring similar to human Testicular Dysgenesis Syndrome, and in fetal life a substantial reduction in anogenital distances.	Not stated.	Variability and Uncertainty in Toxicology of Chemicals in Food, Consumer Products and the Environment March 2007 TOX/2003/09 COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD, CONSUMER PRODUCTS AND THE ENVIRONMENT ADVERSE TRENDS IN DEVELOPMENT OF THE MALE REPRODUCTIVE SYSTEM - POTENTIAL CHEMICAL CAUSES 2003 and annual report 2006)	<a href="http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf">http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf</a> also in <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> referring to SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a> (Other sites with no dose data <a href="http://cot.food.gov.uk/pdfs/vutreportmarch2007.pdf">http://cot.food.gov.uk/pdfs/vutreportmarch2007.pdf</a> , <a href="http://cot.food.gov.uk/pdfs/2003-09endocrine.PDF">http://cot.food.gov.uk/pdfs/2003-09endocrine.PDF</a> , <a href="http://cot.food.gov.uk/pdfs/cotsection06.pdf">http://cot.food.gov.uk/pdfs/cotsection06.pdf</a> )
		There are also recent DBP data from US NTP dietary rat study using a range of doses. Males were exposed to DBP via their mothers throughout pregnancy and lactation and subsequently directly via the diet until adult. Effects on adult testis weight and histopathological lesions shown at doses of 570 mg/kg bw/day and above, with a no-effect level of 250 mg/kg bodyweight/day	testes	Jul 1996 STATEMENT ON PHTHALATES IN INFANT FORMULAE	<a href="http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf">http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf</a>
European Chemicals Bureau (ECB)	Rat, 2 generation reproductivity study	LOAEL based on embryotoxic effects in rats. Absence of maternal toxicity in a two-generation reproduction study with a continuous breeding protocol including improved sensitive endpoints and exposure of both sexes. Protocol intended to identify compounds with endocrine activity. 52 mg/kg bw chosen to be consistent with the EU SCTEE; in an assessment of PVC toys and child-care articles, the SCTEE identified the LOAEL of 0.1% in the diet as critical LOAEL for DBP and set it at 52 mg/kg bw (CSTEE, 1998). However, as observed effects more likely from maternal than paternal dosing, 0.1% of diet equates better to 80 mg/kg bw than to 52 mg/kg bw. Lowest NOAEL for this peroxysomal proliferation in rats was 19.9 mg DBP/kg bw, however this effect not considered important in humans (ECETOC, 1992).	Embryonic development and endocrine activity	European Union Risk Assessment Report Volume 29 , 2003 with addendum 2004	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf</a>
European Food Safety Authority (EFSA)	Rat, development and reproductive studies..	Recent rat developmental study, with dietary DBP exposure from late gestation (day 15) to end of lactation (postnatal day 21), showed effects on the development of male and female offspring at relatively low doses. Germ cell development and mammary gland change at 20 mg/kg in the diet (lowest tested dose), NOAEL could not be established.	Germ cell development and mammary glands.	The EFSA Journal (2005) 242, 1-17 Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Material in Contact with Food (AFC) on a request from the Commission related to Di-Butylphthalate (DBP) for use in food contact materials Question N° EFSA-Q-2003-192 Adopted on 23 June 2005 by written procedure	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ei242_dbp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ei242_dbp_en2.pdf?ssbinary=true</a>

Di n butyl phthalate, Di butyl phthalate or DBP		CAS Number:	84-74-2		Assessor A:	Barry Mitcheson, Envirso		Assessor B:	Alison Pugh, Hyder		Final review:	Panel/SF	
					Date	05/05/2009		Date	05/05/2009		Date	26/08/2009	
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	1999	07/04/2009	TDI	0.05	mg/kgbw/day	50						
European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC)	<a href="http://www.ecetoc.org/">http://www.ecetoc.org/</a>	1998	14/04/2009	TDI	100	ug/kg bw/day	100		LOAEL	52	mg/kg bw/day	500	10 inter, 10 intra and 5 as LOAEL
		2001	21/04/2009	LOAEL	52	mg/kg (bw/day)	52		LOAEL	52	mg/kg bw/day	1000	10 inter, 10 intra and 10 as LOAEL (SR2)
ICPS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>		07/04/2009	ADI	0.066	mg/kgbw/day	66		Approximate LOAEL for developmental and reproductive effects in rats observed in the most sensitive studies to date	66	mg/kgbw/day	1000	10 for interspecies, 10 for interindividual variation, 10 for lack of data on a NOAEL. Factor for lack of a NOAEL considered adequate as effects observed at lowest doses moderate and probably reversible.
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009	TDI	52	ug/kg bw/day	52		LOAEL based on Re-evaluation of human-toxicological Maximum Permissible Levels.	52	mg/kg bw/day	1000	10 for LOAEL to NOAEL and 100 for intra and inter species variation
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	17/12/2007	08/04/2009	TDI	0.0625	mg/kg bw/day	62.5		The NOEL for study in mice for teratogenic and fetotoxic effects.	62.5	mg/kgbw/day	1000	10 for intraspecies, 10 for interspecies and 10 for severity of the effect at the LOAEL in the critical study -(teratogenicity) and for database inadequacies (inadequate chronic toxicity and carcinogenicity);factor considered conservative given large variation in doses in the critical study i.e., the LOAEL is 10 times NOEL.
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report 30 June 2001)	39911	Acute-duration oral MRL	0.5	mg/kgbw/day	500		NOAEL from acute study on rats.	50	mg/kgbw/day	100	10 for use of a LOAEL, 10 for extrapolation from animals to humans, 10 for human variability
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/dinking">http://www.epa.gov/waterscience/criteria/dinking</a>	Last updated on Thur	08/04/2009	Reference to IRIS									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/08/1990 (databse	08/04/2009	Reference dose	1E-1	mg/kg/day	100	Low	NOAEL from Increased mortality Rat Subchronic to Chronic, Oral in Bioassay by Smith, 1953	125	mg/kgbw/day	1000	10 for interspecies variation, 10 sensitive human subpopulations, 10 for both the not chronic study and study deficiencies e.g. only male animals.
Entrez PubMed	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">http://www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>	Date of paper 2007 (abstract only viewed)	20/04/2009	TDI	10	ug/kg bw/day	10						
		Date of paper 2007 (abstract only viewed)	20/04/2009	TDI	10	ug/kg bw/day	10						
TDI inhal					Recommended TDIinhal	CLEA Units	Justification						
					10	ug.kg-1.d-1	Based on ECB study reporting including both local and systemic effects. (Note: value selected is higher than systemic effects based on oral exposure).						
Organisation		Last Updated		Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Drinking Water Inspectorate (DWI)	<a href="http://www.dwi.gov.uk/">http://www.dwi.gov.uk/</a>	31-Mar-09	31-Mar-09										

**Di n butyl phthalate, Di butyl phthalate or DBP**

Scientific Committee on Food (SCF) pre 2002	Rat, 90 day and 1 year oral, reproduction and teratogenicity.	Limited 90-day and 1 year oral rat studies oral reproduction and tetragenicity studies, limited mutagenicity studies (RIVM May 1998). Needed : tests for gene mutation and if migration exceeds 0.05mg/kg 28 oral study and peroxisome proliferation study too.		Compilation of the Evaluations of the scientific committee on food on certain monomers and additives used in the manufacture of plastics materials intended to come into contact with food Stuffs Until 21 March 1997 SCF 1999	<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf</a>
European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC)	Rat, 2 generation reproductive	Reduced pup weights observed in a 2 generation reproductive study with rats	Reduced pup weights	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Phthalate migration from soft PVC toys and child care articles Opinion expressed at the CSTEE third plenary meeting Brussels 24 April 1998	<a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf</a>
	Rat, 2 generation reproductive	2 generation rat study in evaluation of risk of reproductive toxicity. - male reproductive system considered to be main target. Also details a NOAEL (50mg/kg bw/day) and LOAEL (100mg/kg bw/day) for 1 generation study.	Reproductive system	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Opinion of the results of the Risk Assessment Report of Dibutylphthalate. 23rd plenary meeting Brussels, 24 April 2001	<a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out96_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out96_en.pdf</a>
ICPS Environmental Health Criteria (EHC) Monographs	Rat, reproductive, fertility, developmental	NB. The severe, possibly irreversible, teratogenic, testicular and epididymal effects were only observed at the highest dose levels, which also produced other signs of toxicity. Because DBP is rapidly metabolized and eliminated, with no evidence of accumulation, no additional factor was incorporated for lack of data on chronic effects.	Reproductive fertility	INTERNATIONAL PROGRAMME ON CHEMICAL SAFETY ENVIRONMENTAL HEALTH CRITERIA 189 Di-n-butyl Phthalate	<a href="http://www.inchem.org/documents/ehc/ehc/ehc189.htm">http://www.inchem.org/documents/ehc/ehc/ehc189.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Rat, two generation	Based on embryotoxic effects in rats in the absence of maternal toxicity in a two-generation reproduction study.	Embryonic development.	Re-evaluation of human toxicological maximum permissible levels (Baars 2001) Report no. 711701025, available at <a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a> , National Institute for Public Health and the Environment, Bilthoven, The Netherlands. (Also used in Dust evaluation report	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Values	Mice, development and teratogenic study	62.5 mg/kg bw/d is the lowest reported NOEL in an adequate study (for fetotoxic and teratogenic effects in mice observed at the next highest dose) (Hamano et al., 1977). The number of live offspring was decreased, incidence of external defects (spina bifida, exencephaly, cleft palate, non-closing eyelid) and skeletal anomalies (insignificantly) were increased in the offspring of mice administered 625 mg/kg bw/d throughout gestation. At this highest dose, an increase in kidney weight in the mothers was reported.	Fetotoxic and teratogenic effects in mice observed at the next highest dose	Dibutyl Phthalate - PSL1	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-isp1/phthalate_dibutyl_phthalate/phthalate_dibutyl_phthalate_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-isp1/phthalate_dibutyl_phthalate/phthalate_dibutyl_phthalate_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Acute study on rats	Dose-dependent alterations in androgen-regulated male reproductive development in rats exposed during late gestation. Developmental: Increased incidence of retained areolas and nipple in the male offspring of rats exposed to 100 mg/kg/day; no effects observed at 50 mg/kg/day. The systemic toxicity of di-n-butyl phthalate has not been adequately assessed.	Development of male offspring	TOXICOLOGICAL PROFILE FOR DI-n-BUTYL PHTHALATE (refers to Mylchreest E, Wallace DG, Cattley RC, et al. 2000).	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp135.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp135.pdf</a>
USEPA Health Advisors					
USEPA Integrated Risk Information System (IRIS)	Rat, subchronic, oral	NOAEL: 0.25% of diet (125 mg/kg/day) LOAEL: 1.25% of diet (600 mg/kg bw/day)	Increased mortality Rat Subchronic to Chronic, Oral	Refers to BioassaySmith, 1953	<a href="http://www.epa.gov/ncea/iris/subst/0038.htm">http://www.epa.gov/ncea/iris/subst/0038.htm</a>
Entrez PubMed		TDI defined by the European Union - paper not seen.		Di-n-butylphthalate and butylbenzylphthalate - urinary metabolite levels and estimated daily intakes: pilot study for the German Environmental Survey on children. J Expo Sci Environ Epidemiol 2007 Jul; 17(4): 378-87 Epub 2006 sep 27	<a href="http://www.ncbi.nlm.nih.gov/pubmed/17006438?ordinalpos=2&amp;itool=EntrezSystem2.PEntrez.Pubmed.ResultsPanel.Pubmed.DefaultReportPanel.Pubmed.RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/17006438?ordinalpos=2&amp;itool=EntrezSystem2.PEntrez.Pubmed.ResultsPanel.Pubmed.DefaultReportPanel.Pubmed.RVDocSum</a>
		value from European Food Safety Authority (EFSA) - different to the one found on EFSA website above		Internal phthalate exposure over the last 2 decades - a retrospective human biomonitoring study. Int J Hyg Environ Health 2007 May 210 (3-4): 319-33	<a href="http://www.ncbi.nlm.nih.gov/pubmed/17400024?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.ResultsPanel.Pubmed.DefaultReportPanel.Pubmed.RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/17400024?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.ResultsPanel.Pubmed.DefaultReportPanel.Pubmed.RVDocSum</a>
<b>TDI inhal</b>					
Organisation	Study type	Description	Response	Reference	Web link
Drinking Water Inspectorate (DWI)					

Di n butyl phthalate, Di butyl phthalate or DBP	CAS Number:	84-74-2	Assessor A:	Barry Mitcheson, Enviroso	Assessor B:	Alison Pugh, Hyder	Final review:	Panel/SF
			Date	05/05/2009	Date	05/05/2009	Date	26/08/2009

Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>		31/03/2009										
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>	Friday 5 August 2005 (Or	06/04/2009	WEL and STEL	8 hrs - 5, 15 mins - 10	mg.m-3							
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search: 1994 Review of report by MS Technical Experts finalised: 1999 Final report: 2003	07/04/2009	NOAEC of 509mg/m3 for systemic effects and 1.18 LOAEC for local effects	0.012 for local effects (1.616 for systemic effects)	mg/kg bw/day	12 and 1616	Note UF for workers not for children	For local effect an effect was seen at lowest dose (11.18 mg/m3) which is a LOAEC . For systemic effects, no effects observed at highest dose (509 mg/m3) which is a NOAEC.	1.18 and 509	mg/m3	27 for local effects (and 90 for systemic effects)	Interspecies x 3, Intraspecies x 3, experimental conditions vs worker's exposure pattern, Type of critical effect x 1, dose-response curve x 1, Confidence of the database x 3. Total UF = 27
Joint FAO/WHO Meeting on Pesticide Residues (JMPR)	<a href="http://www.who.int/ipcs/food/impr/en/">http://www.who.int/ipcs/food/impr/en/</a>		08/04/2009										
JMPR 2	<a href="http://inchem.org/pages/impr.html">http://inchem.org/pages/impr.html</a>		08/04/2009										
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009										
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/dinking">http://www.epa.gov/waterscience/criteria/dinking</a>	Last updated on Thursday, March 26th, 2009.	08/04/2009	Reference to IRIS									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	26/7/1990 (database last commented in 1998)	08/04/2009										

ID oral													
					Recommended ID oral	Units			Justification				
					n/a				Weight of evidence indicates not carcinogenic				

Organisation		Last Updated		Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating			Basis
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	Friday 5 August 2005 (One site date not given)	31/03/2009	Site refer to endocrine disruptors not to carcinogenicity								
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search: 1994 Review of report by MS Technical Experts finalised: 1999 Final report: 2003	07/04/2009	No adequate long-term toxicity and/or carcinogenicity studies in animals as well as humans are available								
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009	"No TDI given no long term studies for carcinogenic effects of DBP, in human or in laboratory animals".								
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	17/12/2007	08/04/2009	Group VI ("Unclassifiable with Respect to its Carcinogenicity to Humans")								

Di n butyl phthalate, Di butyl phthalate or DBP

Food Standards Agency (FSA)		Not data on inhalation dose. Reference make to endocrine disruptors. Site relates to contact with food			<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
Health and Safety Executive (HSE)			Risk Phrases refer to R60 and R61 (harm fertility and harm the unborn child) and R50 toxic to aquatic organisms	HSC/04/06 Annex C	<a href="http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf">http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf</a>
European Chemicals Bureau (ECB)	Rat, 28-day inhalation	Study in line with current good practise. Further notes on UF: Because an inhalation study is used a factor for allometric scaling is not necessary, and a factor 3 is applicable. A factor for extrapolation of exposure duration is not considered necessary since it is assumed that exposure duration will only have influence on the severity of the effects and not on the level of toxicity c) A factor 3 is introduced for the extrapolation of a LOAEC to a NOAEC	Upper respiratory tract (local effect)	European Union Risk Assessment Report Volume 29 , 2003 with addendum 2004. Refers to Gamer et al., 2000.	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf</a>
Joint FAO/WHO Meeting on Pesticide Residues (JMPR)		reference to phthalates only relate to DMP as solvent for dermal test and DEHP and an interference			
JMPR 2		reference to phthalates only relate to DMP as solvent for dermal test and DEHP and an interference			
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels		Baars et al states that inhalation not considered relevant due to low volatility. The dust paper uses the oral EFSA value given above		re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
USEPA Health Advisors					
USEPA Integrated Risk Information System (IRIS)		The health effects data for dibutyl phthalate were reviewed by the U.S. EPA RfD/RfC Work Group and determined to be inadequate for derivation of an inhalation RfC.			<a href="http://www.epa.gov/ncea/iris/subst/0038.htm">http://www.epa.gov/ncea/iris/subst/0038.htm</a>
<b>ID oral</b>					
<b>Organisation</b>	<b>Study type</b>	<b>Description</b>	<b>Response</b>	<b>Reference</b>	<b>Web link</b>
Food Standards Agency (FSA)					<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
European Chemicals Bureau (ECB)				European Union Risk Assessment Report Volume 29 , 2003 with addendum 2004	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels				re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Values		Carcinogenicity is potentially the most sensitive endpoint. The weight of available data in in vitro assays indicates that dibutyl phthalate is not genotoxic. No human epidemiological studies to assess carcinogenicity and available data considered inadequate to assess the carcinogenicity animals.		Dibutyl Phthalate - PSL1	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-isp1/phthalate_dibutyl_phthalate/phthalate_dibutyl_phthalate_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-isp1/phthalate_dibutyl_phthalate/phthalate_dibutyl_phthalate_3-eng.php</a>

Di n butyl phthalate, Di butyl phthalate or DBP	CAS Number:	84-74-2	Assessor A:	Barry Mitcheson, Enviroso	Assessor B:	Alison Pugh, Hyder	Final review:	Panel/SF
	Date	05/05/2009	Date	05/05/2009	Date	26/08/2009		

USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/02/1990 (database last commented in 1998)	08/04/2009	Classification — D; not classifiable.  Basis — Pertinent data regarding carcinogenicity was not located in the available literature.									
<b>ID inhal</b>					<b>Recommended Id inhal</b>	<b>Units</b>	<b>Justification</b>						
					n/a		Weight of evidence indicates not carcinogenic						
<b>Organisation</b>		<b>Last Updated</b>		<b>Non threshold effects?</b>	<b>Basis</b>	<b>Health criteria type</b>	<b>Value</b>	<b>Units</b>	<b>Confidence rating</b>				<b>Basis</b>
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>		06/04/2009	HSC/04/06 Annex C All three listed. WEL 5mg/m3 and STEL 10mg/m3. Risk Phrases refer to R60 and R61 (harm fertility and harm the unborn child) and R50 Very toxic to aquatic organisms									
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search: 1994 Review of report by MS Technical Experts finalised: 1999 Final report: 2003	07/04/2009	No adequate long-term toxicity and/or carcinogenicity studies in animals as well as humans are available									
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>		07/04/2009										
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2001 (replaced 2008)	08/04/2009	"No TDI given no long term studies for carcinogenic effects of DBP, in human or in laboratory animals".									
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	17/12/2007	08/04/2009	Group VI ("Unclassifiable with Respect to its Carcinogenicity to Humans")									
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/02/1990 (database last commented in 1998)	08/04/2009	Classification — D; not classifiable.									

**Di n butyl phthalate, Di butyl phthalate or DBP**

USEPA Integrated Risk Information System (IRIS)					<a href="http://www.epa.gov/ncea/iris/subst/0038.htm">http://www.epa.gov/ncea/iris/subst/0038.htm</a>
ID inhal					
<b>Organisation</b>	<b>Study type</b>	<b>Description</b>	<b>Response</b>	<b>Reference</b>	<b>Web link</b>
Health and Safety Executive (HSE)					<a href="http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf">http://www.hse.gov.uk/aboutus/meetings/hscarchive/2004/091104/c06c.pdf</a>
European Chemicals Bureau (ECB)				European Union Risk Assessment Report Volume 29 , 2003 with addendum 2004	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf</a>
Scientific Committee on Food (SCF) pre 2002		Available limited 90-day and 1 year oral rat studies oral reproduction and tetragenicity studies, limited mutagenicity studies (RIVM May 1998). Needed : tests for gene mutation and if migration exceeds 0.05mg/kg 28 oral study and peroxisome proliferation study too.		Compilation of the Evaluations of the scientific committee on food on certain monomers and additives used in the manufacture of plastics materials intended to come into contact with food Stuffs Until 21 March 1997 SCF 1999	<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels		Baars et al states that inhalation not considered relevant due to low volatility. The dust paper uses the oral EFSA value given above		re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Values		Inhalation not specifically addressed. The weight of available data in in vitro assays indicates that dibutyl phthalate is not genotoxic. Carcinogenicity is potentially the most sensitive endpoint. No human epidemiological studies to assess carcinogenicity and available data considered inadequate to assess the carcinogenicity animals.		Dibutyl Phthalate - PSL1	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/phthalate_dibutyl_phtalate/phthalate_dibutyl_phtalate_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psl1-lsp1/phthalate_dibutyl_phtalate/phthalate_dibutyl_phtalate_3-eng.php</a>
USEPA Integrated Risk Information System (IRIS)		Basis — Pertinent data regarding carcinogenicity was not located in the available literature.			<a href="http://www.epa.gov/ncea/iris/subst/0038.htm">http://www.epa.gov/ncea/iris/subst/0038.htm</a>

Di n butyl phthalate	CAS 84-74-2	Assessor A: Date	Barry Mitcheson, Enviros 05/05/2009	Assessor B: Date	Alison Pugh, Hyder 05/05/2009	Final review: Date	Panel/SF 26/08/2009
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MDI		Recommended MDI oral	Units	Justification: Large range of values for oral exposure. A mid range value (towards the upper end) which is referenced in Canada, and 2 of the recent German studies. Exposure may be greater for infants due to infant milk, but will be for a relatively short			
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Food Standards Agency	1993	Diet	31	ug day-1	Mean 0.013mg/person/day High end 0.031mg/person per day)	82: MAFF UK - Phthalates in Food (March 1996) Table 2: Estimated mean and high level (97.5th percentile) intakes of individual phthalates from carcass meat, poultry, eggs and milk, based on the analysis of 1993 Total Diet Study samples	<a href="http://www.food.gov.uk">www.food.gov.uk</a> <a href="http://archive.food.gov.uk/maff/archive/food/infsheet/1996/no82/table2.htm#Table2">http://archive.food.gov.uk/maff/archive/food/infsheet/1996/no82/table2.htm#Table2</a>
	1998	Infant milk	13.44	ug day-1	At birth 2.4ug/kgbw/day to 1.4ug/kgbw/day at six months, converts using 5.6kg bodyweight for 0-1 year old	Food Surveillance sheet Number 168 December 1998 MAFF UK - PHTHALATES IN INFANT FORMULAE - FOLLOW-UP SURVEY Table 2: Concentrations and Estimated Average. <a href="http://archive.food.gov.uk/maff/archive/food/infsheet/1998/no168/tables.htm">http://archive.food.gov.uk/maff/archive/food/infsheet/1998/no168/tables.htm</a> Exposure to Individual and Total Phthalates of Infants at Birth and Six Months of Age from Retail Infant Formulae	
Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	12/04/2009	No Data				TOX/2004/25 COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD, CONSUMER PRODUCTS AND THE ENVIRONMENT- TOXICOLOGICAL EVALUATION OF A PILOT STUDY FOR A BREAST- MILK ARCHIVE	<a href="http://www.cot.food.gov.uk">www.cot.food.gov.uk</a>
European Chemicals Bureau (ECB)	12/04/2009	Food, air and water	25.13	ug day-1	3.59x10-4 mg/kgbw/day based on regional modelling using EUSES Calculation for adults using 70kg body weight	European Union Risk Assessment Report Volume 29 , 2003 with addendum 2004	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a> <a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf</a>
	12/04/2009	Food, air and water	2.872	ug day-1	3.59x10-4 mg/kgbw/day based on regional modelling using EUSES Calculation for children using 8kg body weight	European Union Risk Assessment Report Volume 29 , 2003 with addendum 2004	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dibutylphthalatereport003.pdf</a>
European Food Safety Authority (EFSA)	12/04/2009	Diet	31	ug day-1	The limited available data on DBP concentration in foods and diets in the UK and Denmark were used to provide an estimation of dietary exposure. In the UK, mean and high (97.5th percentile) intakes of DBP from dietary sources were estimated to be respectively 0.013 and 0.031 mg/person/day in the adult population (equivalent to 0.2 and 0.5 µg/kg bw/day) considering a 60 kg adult.	The EFSA Journal (2005) 242, 1-17 Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Material in Contact with Food (AFC) on a request from the Commission related to Di-Butylphthalate (DBP) for use in food contact materials Question N° EFSA-Q-2003-192 Adopted on 23 June 2005 by written procedure	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a> <a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej242_dbp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej242_dbp_en2.pdf?ssbinary=true</a>
	12/04/2009	Diet	29 for adults, in first study and in second study 112 for adults, 64 for 1-6 children and 3.5 * bodyweight of a 7-14 year old child	ug day-1	A Danish study estimated mean DBP exposure between 0.13 to 0.29 mg/day, i.e. 1.8 to 4.1 µg/kg bw/day, for a 70 kg adult. Based on maximum dietary DBP concentrations, exposure at high percentiles estimated as 0.72 mg/day equivalent to 10.2 µg/kg bw/day. A further Danish study, found main dietary sources to be root crops (83%) and leaf crops (13%). The oral daily intake for Denmark was estimated at 1.6 µg/kg bw/day in adults, 8 µg/kg bw/day in children aged 1 to 6 years, and 3.5 µg/kg bw/day in children aged 7 to 14 years.	The EFSA Journal (2005) 242, 1-17 Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Material in Contact with Food (AFC) on a request from the Commission related to Di-Butylphthalate (DBP) for use in food contact materials Question N° EFSA-Q-2003-192 Adopted on 23 June 2005 by written procedure	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej242_dbp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej242_dbp_en2.pdf?ssbinary=true</a>
	12/04/2009	Infant milk formula and breast milk	91.84 for <six months 36.96 to 44.24 for six months (note body weight assumed to be 5.6kg (possibly large for <six months)	ug day-1	Based on the detection limit, intake from infant formulae would be <16.4 µg/kg bw/day in infants <6 months and 6.6 µg/kg bw/day in infants > 6 months. For infants >6 months, ready-to-use baby foods were also taken into account and the exposure was therefore estimated as <7.9 µg/kg bw/day.	The EFSA Journal (2005) 242, 1-17 Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Material in Contact with Food (AFC) on a request from the Commission related to Di-Butylphthalate (DBP) for use in food contact materials Question N° EFSA-Q-2003-192 Adopted on 23 June 2005 by written procedure	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej242_dbp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej242_dbp_en2.pdf?ssbinary=true</a>
European Centre for Ecotoxicology and Toxicology of Chemicals (ECETOC)	22/04/09 (1998)	human intake	2170 (assumes 70kg bw)	ug day-1	31ug/kg bw/day, maximum likely human intake in UK in adults (based on WHO - EHC paper)	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Phthalate migration from soft PVC toys and child care articles Opinion expressed at the CSTEE third plenary meeting Brussels 24 April 1998	<a href="http://www.ecetoc.org/">www.ecetoc.org/</a> <a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out12_en.pdf</a>
	22/04/09 (2001)	repeated exposure	2100ug/day (assumes 70kg bw)	ug day-1	0.03mg/kg/day, exposure from DBP containing products - adult exposure for repeated exposure	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE). Opinion of the results of the Risk Assessment Report of Dibutylphthalate. 23rd plenary meeting Brussels, 24 April 2001	<a href="http://ec.europa.eu/health/ph_risk/committees/sct/documents/out96_en.pdf">http://ec.europa.eu/health/ph_risk/committees/sct/documents/out96_en.pdf</a>
IPCS Environmental Health Criteria (EHC) Monographs	22/04/2009 (1997)	food and drinking water	2170ug/day (assumes 70kg bw)	ug day-1	31ug/kgbw/day, Intake from food for the UK likely to be 2mg/person. Drinking water is <0.02ug/kg bw/day. Possible mis-quoting of MAFF source.	International Programme on Chemical Safety, Environmental Health Criteria 189 Di-n-butyl Phthalate, World Health	<a href="http://incchem.org/pages/ehc.html">http://incchem.org/pages/ehc.html</a> Organisation (1997) <a href="http://incchem.org/documents/ehc/ehc189.htm">http://incchem.org/documents/ehc/ehc189.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	12/04/2009	All media primarily food	Dust report gives 210 to 1120 for adults and about 120 to 260ug/day for children. MPR report equated to 350 -	ug day-1	No DBP specific data - reference to total phthalates based on DEHP and butyl benzyl phthalate. Dust data report gives Background value of DEHP for adults is between 3 and 16 µg/kg/day and Background value of DEHP for children is between 12 and 26 µg/kg/day.	Re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a> <a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> & <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)
Health Canada Toxicological Reference Values	12/04/2009	exposure mostly food (but indoor air can be significant)	1.9 ug/kg bw/day for adults equivalent to 133ug/day 5ug/kg bw/day equivalent to about 40-50ug/day	ug/day	Substrate/Medium Estimated Intake (µg/[kg(b.w.)-day])  0 to 0.5 yrb      0.5 to 4 yr      5 to 11yrd      12 to 19 yre      20 to 70 yrf <i>Drinking water</i> 0.1                      0.06                      0.03                      0.02                      0.02 <i>Food</i> 1.6                      4.1                      3.2                      1.4                      1.1	17/12/2007 Dibutyl Phthalate - PSL1 <a href="http://www.hc-sc.gc.ca/ewh-scmt/pubs/contaminants/psl1-lsp1/phthalate_dibutyl_phthalate/phthalate_dibutyl_phthalate_3-eng.php">http://www.hc-sc.gc.ca/ewh-scmt/pubs/contaminants/psl1-lsp1/phthalate_dibutyl_phthalate/phthalate_dibutyl_phthalate_3-eng.php</a>	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>



Di n butyl phthalate	CAS 84-74-2	Assessor A:	Barry Mitcheson, Enviros	Assessor B:	Alison Pugh, Hyder	Final review:	Panel/SF
		Date	05/05/2009	Date	05/05/2009	Date	26/08/2009
Toxicological Data Network (TOXNET)	12/04/2009	Air	Different value using 20m3 per day gives <b>0-0.12ug/day</b>	ug day-1	HSDB database AIR INTAKE: (assume 0-6 ng/cu m) 0-400 ng(1); WATER INTAKE: (assume 0-2.5 ug/L(2)) 20 ng-10,000 ng; FOOD INTAKE: insufficient data(SRC).	[(1) Kelly TJ et al; Environ Sci Technol 28: 378-87 (1994) (2) Davies K; Adv Environ Sci Technol 23: 525-40 (1990) ]**PEER REVIEWED**	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>



Di-n-octyl phthalate	CAS Number: 117-84-0	Assessor A: B Mitcheson, Enviro	Assessor B: S Cole, URS	Final review: Panel/SF
		Date 05/05/2009	Date 10/08/2009	Date 09/09/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	NR	No information relating to potential carcinogenicity. TDloral applied to oral, dermal and inhalation routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		No information relating to potential carcinogenicity. Insufficient information to derive TDlinhal, route-to-route from TDloral used.

TDI oral	Recommended TDI oral	Units	Justification
	50	ug.kg-1.d-1	Two values available: (1) 50 ug/kg/d is the temporary group restriction for phthalates with no specific TDI set by the SCF. This is based on dose-response data for DEHP (2) approx 400 ug/kg/d based on a sub chronic study by Poon. The sub chronic study is not considered of sufficient duration for derivation of a TDloral and therefore preference is given to the SCF group restriction of 50 ug/kg/d as the TDloral for di-n-octylphthalate. This assumes that the threshold toxicity of this compound is equivalent to that of DEHP.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Drinking Water Inspectorate (DWI)	<a href="http://www.dwi.gov.uk/">http://www.dwi.gov.uk/</a>		31-Mar-09	No dose data identified - searched for plasticiser, phthalate, dicarboxylic. Note that tests for plastic pipes must comply with BS 6920 which includes a flavour and odour test										
		31-Mar-09												
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>		31/03/2009	Provisional TDI for all phthalate esters in contact with food	50	ug/kg/day	50	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown
		Friday 5 August 2005 (O												
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	<a href="http://cot.food.gov.uk/">http://cot.food.gov.uk/</a>		06/04/2009	Provisional TDI for all phthalate esters in contact with food	0.05	mg/kg.bw/day	50	The Committee was aware that new evidence on the reproductive effects of phthalates has been published since these TDIs were set.	NOAEL	Unknown	Unknown	100	Unknown	Unknown
		29/04/08 (uploaded infant milk formula file from July 2006)												
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	16 December 1994 report	07/04/2009	Provisional TDI for all phthalate esters in contact with food	0.05	mg/kg.bw/day	50	Unknown	Based on extrapolated NOAEL for DEHP	No info	No info	No info	No info	No info
EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE)	<a href="http://ec.europa.eu/health/ph_risk/committees/sct/sct_en.htm">http://ec.europa.eu/health/ph_risk/committees/sct/sct_en.htm</a>		16/05/2009	TDI	0.37	mg/kg.bw/day	370	Unknown	NOAEL	36.8	mg/kg.bw/day	100	Assumed margin of safety required for calculating TDI from NOAEL in context of exposure to phthalates from children sucking plastic toys	Subchronic 13week oral study in rats
		24-Apr-98												
Joint FAO/WHO Meeting on Pesticide Residues (JMPR)	<a href="http://www.who.int/ipcs/food/jmpr/en/">http://www.who.int/ipcs/food/jmpr/en/</a>		08/04/2009	Reference to phthalates only relate to DMP as solvent for dermal test and DEHP and an interference										
JMPR 2	<a href="http://linchem.org/pages/jmpr.html">http://linchem.org/pages/jmpr.html</a>		08/04/2009	Reference to phthalates only relate to DMP as solvent for dermal test and DEHP and an interference										
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	1993	16/05/2009	Report identified with reference to tox studies but no TDI derived										

## Di-n-octyl phthalate

TDI oral
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Organisation	Description	Target organ/Critical Effect	Reference	Web link
Drinking Water Inspectorate (DWI)				
Food Standards Agency (FSA)	Refers to a provisional TDI of 50ug/kgbw/day for all phthalate esters in contact with food. Also Plastic Materials and Articles In Contact With Food (England) Regulation 2008 look at specific limits on phthalate transfer into food.	Unknown	Unknown	<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates</a> ; <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> ; <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a>
Committee on the Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	These e temporary "group restriction" of 0.05 mg/kg bodyweight/day set by the (Scientific Committee on Food (SCF) for those phthalates for which further toxicity testing is required. The Committee notes that TDIs are derived from doses which produce no effect in animal studies	Unknown	Jul 2006 STATEMENT ON PHTHALATES IN INFANT FORMULAE. Based on the Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a> (Other sites Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment Risk Assessment of Mixtures of Pesticides and Similar Substances synergistic effects) <a href="http://cot.food.gov.uk/pdfs/reportindexed.pdf">http://cot.food.gov.uk/pdfs/reportindexed.pdf</a>	<a href="http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf">http://cot.food.gov.uk/pdfs/cotstatementphthalates96.pdf</a> also in <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> referring to SCF (1996). Phthalates in infant formulae (Opinion expressed on 7 June 1996). Reports of the Scientific Committee on Food, 36th Series. Available at: <a href="http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html">http://europa.eu.int/comm/food/fs/sc/scf/reports_en.html</a>
Scientific Committee on Food (SCF) pre 2002	Group restriction peroxisome proliferation, reproductive study, inadequate 90day oral study and Ames test available	Unknown		<a href="http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf">http://ec.europa.eu/food/fs/sc/scf/reports/scf_reports_42.pdf</a>
EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE)	DNOP was shown to cause mild microscopic changes in the liver (endothelial nuclear prominence, nuclear hyperchromicity, anisokaryosis) and thyroid (reduced follicle size, reduced colloid density) at 5000 ppm in diet. NOAEL = 500 ppm which is equivalent to 36.8 mg/kg bw/day for male rats (Poon et al., 1997).	Liver and thyroid	EU Scientific Committee on Toxicity, Ecotoxicity and the Environment (CSTEE. Phthalate migration from soft PVC toys and child-care articles Opinion expressed at the CSTEE third plenary meeting Brussels, 24 April 1998 which cites Poon R, Lecavalier, P, Mueller, R, Valli, VE, Procter BG, Chu I (1997). Subchronic Oral toxicity of di-n-octyl phthalate and di(2-ethylhexyl) phthalate in the rat. Fd Chem Toxicol 35, 225-239.	<a href="http://ec.europa.eu/health/ph_rsk/committees/sct/documents/out12_en.pdf">http://ec.europa.eu/health/ph_rsk/committees/sct/documents/out12_en.pdf</a>
Joint FAO/WHO Meeting on Pesticide Residues (JMPR)				
JMPR 2				
Health Canada Toxicological Values				<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/dinocylphthalate_phtalatedioctyle/dinocylphthalate_phtalatedioctyle_2-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/dinocylphthalate_phtalatedioctyle/dinocylphthalate_phtalatedioctyle_2-eng.php</a>

Di-n-octyl phthalate		CAS Number: 117-84-0		Assessor A: B Mitcheson, Enviro	Assessor B: S Cole, URS	Final review: Panel/SF						
		Date	05/05/2009	Date	10/08/2009	Date	09/09/2009					
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	September 1997	16/05/2009	Intermediate duration MRL	0.4 mg/kg.bw/day	400	Unknown	NOAEL	40.8 mg/kg.bw/day	100	Intermediate [X] 10 for extrapolation from animals to humans [X] 10 for human variability	Poon et al 1995- 13 week diet study on rats

<b>TDI inhal</b>	<b>Recommended TDI inhal</b>	<b>Units</b>	<b>Justification</b>
			insufficient information available to recommend a TDI inhal

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Units	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Drinking Water Inspectorate (DWI)	<a href="http://www.dwi.gov.uk/">http://www.dwi.gov.uk/</a>		31-Mar-09	No dose data identified - searched for plasticiser, phthalate, dicarboxylic. Note that tests for plastic pipes must comply with BS 6920 which includes a flavour and odour test									
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	31-Mar-09	31/03/2009	Not data on inhalation dose. Reference make to endocrine disruptors. Site relates to contact with food									
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>	Friday 5 August 2005 (O	16/05/2009	Page on exposure standards details no drinking water standard, soil standard or air standard									
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search : 2005. Review of report by MS Technical Experts finalised: September 2005. Final report: 2008	07/04/2009										
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>		07/04/2009	No data in EHC131									
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>		16/05/2009										
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	19/04/2007	08/04/2009	No comment on inhalation									
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	08/04/2009	No inhalation MRLs were derived for DOP due to inadequate data for this route of exposure.									

<b>ID oral</b>	<b>Recommended ID oral</b>	<b>Units</b>	<b>Justification</b>
	n/a		Weight of evidence indicates unlikely carcinogenic.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>	Friday 5 August 2005 (O	31/03/2009		Site refer to endocrine disruptors not to carcinogenicity						
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	<a href="http://www.advisorybodies.doh.gov.uk/coc/index.htm">http://www.advisorybodies.doh.gov.uk/coc/index.htm</a>		06/04/2009		No dose data identified.						

**Di-n-octyl phthalate**

<p><b>US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels</b></p>	<p>Groups of 10 male and 10 female Sprague-Dawley rats were maintained on diets containing 0, 5, 50, 500, or 5,000 ppm di-n-octylphthalate (DNOP) in the diet for 13 weeks. The study authors determined that these dietary concentrations corresponded to doses of 0, 0.4, 3.5, 36.8, 350.1 mg/kg/day (males) and 0, 0.4, 4.1, 40.8, 402.9 mg/kg/day (females). The rats were examined daily for clinical signs of toxicity, while food consumption and body weight data were collected weekly. Blood and comprehensive histopathological examinations were performed at the end of the study (although only data on the liver, thyroid, testis, and epididymis were presented).</p>	<p>Liver effects observed in rats administered di-n-octylphthalate in the diet at a concentration of 5,000 ppm; the study authors calculated the doses at this concentration to be 350.1 mg/kg/day (males) and 402.9 mg/kg/day (females) (Peon et al. 1995). The hepatic effects consisted of a significant (p &lt; 0.05) increases in ethoxyresorufin-O-deethylase activity (12-fold, males; 3-fold, females); no significant changes were noted in liver aminopyrine-N-demethylase or aniline hydrolase activities. Also, at 5,000 ppm, histopathological changes in hepatic architecture were noted, including moderate accentuation of zonation and mild-to-moderate increases in perivenous cytoplasmic vacuolation. Mild histological changes in the thyroid were also noted at 5,000 ppm that consisted of reduction in the follicle size and decreased colloid density. No effects were observed at 500 ppm (36.8 mg/kg/day for males and 40.8 mg/kg/day for females).</p>	<p>TOXICOLOGICAL PROFILE FOR DI-N-OCTYLPHTHALATE U.S. DEPARTMENT OF HEALTH AND HUMAN SERVICES. Public Health Service Agency for Toxic Substances and Disease Registry, September 1997</p>	<p><a href="http://www.atsdr.cdc.gov/toxprofiles/tp95.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp95.pdf</a> (&amp; <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)</p>
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**TDI inhal**

Organisation	Description	Response	Reference	Web link
Drinking Water Inspectorate (DWI)				???
Food Standards Agency (FSA)				<p><a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> &amp; <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> &amp; <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (</p>
Health Protection Agency (HPA)			Phthalates (Diisononylphthalate and Di(2-ethylhexyl)phthalate) Incident management, Health Protection Agency 2008	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949</a>
European Chemicals Bureau (ECB)				??????
IPCS Environmental Health Criteria (EHC) Monographs				<a href="http://www.inchem.org/documents/ehc/ehc/ehc131.htm">http://www.inchem.org/documents/ehc/ehc/ehc131.htm</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels			Re-evaluation of maximum permissible levels By Baars et al RIVM 711701025/2001 superseded by RIVM Report 609021064/2008 Exposure to chemicals via house dust A. G. Oomen P. J.C.M. Janssen A. Dusseldorp C. W. Noorlander	<p><a href="http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf">http://www.rivm.nl/bibliotheek/rapporten/609021064.pdf</a> &amp; <a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a> (Baars et al)</p>
Health Canada Toxicological Values			Bis(2-ethylhexyl) Phthalate - PLS1	<p><a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/bis_2_ethylhexyl/bis_2_ethylhexyl_3-eng.php</a></p>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels			TOXICOLOGICAL PROFILE FOR DI-N-OCTYLPHTHALATE U.S. DEPARTMENT OF HEALTH AND HUMAN SERVICES Public Health Service Agency for Toxic Substances and Disease Registry September 1997	<p><a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a> (&amp; <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)</p>

**ID oral**

Organisation	Description	Response	Reference	Web link
Food Standards Agency (FSA)				<p><a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> &amp; <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> &amp; <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF (</p>
Committee on the Carcinogenicity of Chemicals in Food, Consumer Products and the Environment (COC)	Chemicals for which a tumorigenic effect was first observed between 53 and 80 week in rats and/or mice.		CC/01/25 COMMITTEE ON CARCINOGENICITY OF CHEMICALS IN FOOD CONSUMER PRODUCTS AND THE ENVIRONMENT THE MINIMUM DURATION OF CARCINOGENICITY STUDIES IN RATS, November 2001	<a href="http://www.iacoc.org.uk/papers/documents/mindurcarstudy.PDF">http://www.iacoc.org.uk/papers/documents/mindurcarstudy.PDF</a>

Di-n-octyl phthalate		CAS Number:	117-84-0	Assessor A:	B Mitcheson, Enviros	Assessor B:	S Cole, URS	Final review:	Panel/SF
		Date	05/05/2009	Date	10/08/2009	Date	09/09/2009		
European Food Safety Authority (EFSA)	<a href="http://www.efsa.europa.eu/en.html">http://www.efsa.europa.eu/en.html</a>	Report from 2005	07/04/2009	No comment on carcinogenicity					
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>		16/05/2009	No data					
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	16/05/2009	Di-n-octylphthalate has not been classified for carcinogenic effects by the Department of Health and Human Services, the International Agency for Research on Cancer, or the EPA.					

ID inhal	Recommended ID inhal	Units	Justification
	n/a		Weight of evidence indicates unlikely carcinogenic.

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
Food Standards Agency (FSA)	<a href="http://www.food.gov.uk/">http://www.food.gov.uk/</a>		31/03/2009	No data on inhalation doses identified. Site refers to endocrine disruptors not carcinogens.							
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>	Friday 5 August 2005 (O	31/03/2009	Page on exposure standards details no drinking water standard no soil standard or air standard							
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	Date of Last Literature Search : 2005. Review of report by MS Technical Experts finalised: September 2005. Final report: 2008	07/04/2009	No data							
European Food Safety Authority (EFSA)	<a href="http://www.efsa.europa.eu/en.html">http://www.efsa.europa.eu/en.html</a>	Report from 2005	07/04/2009	No data							
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>		07/04/2009	No data							
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	14/01/2009 for MRL page (And report June 2002)	08/04/2009	No studies were located regarding geotaxis effects in humans after inhalation, oral, or dermal exposure to DEHP. As discussed below, DEHP has been extensively tested in a variety of short-term genotoxicity assays with predominantly negative or false-positive results. The weight of evidence from these assays, as well as the tumour initiating/promoting activity studies summarized in Section 3.5.2 (Mechanisms of Toxicity), indicate that DEHP does not induce lesions in nuclear DNA, is not mutagenic/geotaxis, and is not a tumour initiator, but rather that it is a rodent liver mutagen and tumour promoter, and is best characterized as an epigenetic toxicant.							

## Di-n-octyl phthalate

European Food Safety Authority (EFSA)			Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in Contact with Food (AFC) on a request from the Commission related to Bis(2-ethylhexyl)phthalate (DEHP) for use in food contact materials Question N° EFSA-Q-200	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true</a>
International Agency for Research on Cancer (IARC)			International Agency for Research on Cancer (IARC) - Summaries & Evaluations DI(2-ETHYLHEXYL) PHTHALATE (Group 3) VOL.: 77 (2000) (p. 41)	<a href="http://www.inchem.org/documents/iarc/vol77/77-01.html">http://www.inchem.org/documents/iarc/vol77/77-01.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels			TOXICOLOGICAL PROFILE FOR DI-n-OCTYLPHTHALATE U.S. DEPARTMENT OF HEALTH AND HUMAN SERVICES Public Health Service Agency for Toxic Substances and Disease Registry September 1997	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp95.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp95.pdf</a> (& <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)

## ID inhal

Organisation	Description	Response	Reference	Web link
Food Standards Agency (FSA)				<a href="http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/">http://www.food.gov.uk/foodlabelling/packagingbranch/phthalates/</a> & <a href="http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en">http://www.eatwell.gov.uk/healthissues/factsbehindissues/phthalates/?lang=en</a> & <a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a> SCF
Health Protection Agency (HPA)			Phthalates (Diisononylphthalate and Di(2-ethylhexyl)phthalate) Incident management, Health Protection Agency 2008	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1194947324949</a>
European Chemicals Bureau (ECB)			European Union Risk Assessment Report Volume 80 , 2008	<a href="http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf">http://ecb.jrc.ec.europa.eu/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/dehpreport042.pdf</a>
European Food Safety Authority (EFSA)			Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in Contact with Food (AFC) on a request from the Commission related to Bis(2-ethylhexyl)phthalate (DEHP) for use in food contact materials Question N° EFSA-Q-200	<a href="http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true">http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/afc_op_ej243_dehp_en2.pdf?ssbinary=true</a>
International Agency for Research on Cancer (IARC)			International Agency for Research on Cancer (IARC) - Summaries & Evaluations DI(2-ETHYLHEXYL) PHTHALATE (Group 3) VOL.: 77 (2000) (p. 41)	<a href="http://www.inchem.org/documents/iarc/vol77/77-01.html">http://www.inchem.org/documents/iarc/vol77/77-01.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels			Toxicological Profile for Di(2-ethylhexyl)phthalate (DEHP) September 2002 including Reference: David RM, Moore MR, Finney DC, et al. 2000a. Chronic toxicity of di(2-ethylhexyl)phthalate in rats. Toxicol Sci 55:433-443.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp9.pdf</a> (& <a href="http://www.atsdr.cdc.gov/mrls/index.html">http://www.atsdr.cdc.gov/mrls/index.html</a> for MRLs)

<b>Di-n-octyl phthalate</b>	CAS 117-84-0	Assessor A:	B Mitcheson, Enviros	Assessor B:	Simon Cole, URS	Final review:	Panel/SF
		Date	05/05/2009	Date	10/08/2009	Date	09/09/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	Based on NTP comment that DnOP exposure significantly less than DEHP. Thus, exposure assumed not to exceed 3 ug/kg/d. Converted assuming a 70kg adult to 210 ug/d for an adult.
	<b>210</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Food Standards Agency	1993	Diet			Diet data for combined phthalates. Majority appears to be diethylhexylphthalate. (Conc DEHP is the same as Total DOPs for carcass meat and eggs but total DOP in milk is 2.6mg/kg but DEHP is 0.3mg/kg)	82: MAFF UK - Phthalates in Food (March 1996) Table 2: Estimated mean and high level (97.5th percentile) intakes of individual phthalates from carcass meat, poultry, eggs and milk, based on the analysis of 1993 Total Diet Study samples.	<a href="http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/table2.htm#Table2">http://archive.food.gov.uk/maff/archive/food/infosheet/1996/no82/table2.htm#Table2</a>
Committee on Toxicity of Chemicals in Food, Consumer Products and the Environment (COT)	12/04/2009				There may be stability issues with the phthalate analysis. The phthalate data previously presented to the COT are therefore considered to be unreliable. This may cast doubt on the FSA data from 1993 and 1998)	COMMITTEE ON TOXICITY OF CHEMICALS IN FOOD, CONSUMER PRODUCTS AND THE ENVIRONMENT. TOXICOLOGICAL EVALUATION OF A PILOT STUDY FOR A BREAST MILK ARCHIVE. TOX/2004/14. April 2004	<a href="http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf">http://cot.food.gov.uk/pdfs/TOX-2004-14.pdf</a>
SCIENTIFIC COMMITTEE ON CONSUMERS PRODUCTS (SCCP)	16/05/2009		not detected in study			Request for a scientific opinion: Phthalates in Cosmetics	<a href="http://ec.europa.eu/health/ph_risk/committees/04_sccp/docs/sc_cp_q_156.pdf">http://ec.europa.eu/health/ph_risk/committees/04_sccp/docs/sc_cp_q_156.pdf</a>
		Leaching from toys	296	ug day-1			
Toxicological Data Network (TOXNET)	12/04/2009	Water	0.0728	mg/year	Average Daily Intake: The estimated mean human exposure to dioctyl phthalate via drinking water in Toronto, Canada is 0.0728 mg/year	Davies K; Adv Environ Sci Technol 23: 525-40 (1990)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
Entrez PubMed	12/04/2009	Comment on overall exposure	< 3	ug/kg/d	The available data do not allow the confident estimation of DnOP exposures to the general population. However, a comparison of production volumes for DnOP-containing compounds versus those that contain DEHP suggests that human exposure to DnOP is well below the exposure estimate for DEHP of 3–30 µg/kg bw/day. Exposures may be higher in children due to dietary preferences or mouthing of DnOP-containing articles	NTP-CERHR Monograph on the Potential Human Reproductive and Developmental Effects of Di-n -Octyl Phthalate (DnOP) May 2003	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>

<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	Midpoint concentration from ATSDR data (0.5 ng/m3) x assumed adult inhalation rate of 20 m3/d / 1000 ng/ug gives an estimated MDI of 0.01 ug.d-1.
	<b>0.01</b>	<b>ug day-1</b>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	12/04/2009	Air	0.06 to 0.94	ng/m3	Di-n-octyl phthalate detected in 5 of 7 ambient air samples taken in Feb 1984 Portland, Oregon, USA. Detected concs ranged from 0.06 to 0.94 ng/m3.		<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>

Substance:		Di-n-octyl phthalate		CAS Number:	117-84-0		Assessor A:	J Thornton, Golder Associates		Assessor B:	D Dyson, URS		Final review:	Panel/SF																
Chemical Formula:		C24H38O4		Phase at Ambient Temperature:	Liquid		Date:	28-May-09		Date:	26-Mar-09		Date:	09/09/2009																
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al, 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000		
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	390.56	n/a	Median value from consistent range		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
						Average	No data	#DIV/0!	n/a	390.557	390.557	n/a	390.56	390.56	n/a	No data	#DIV/0!	n/a	390.57	390.57	n/a	Not Reviewed	#DIV/0!	n/a	390.5561	390.5561	n/a	No data	#DIV/0!	n/a
						Geomean	No data	Insert Values		No data	Insert Values		5.57E-01	0.557					1.41E-12	1.4286E-07		Not Reviewed	Insert Values		No data	Insert Values		No data	Insert Values	
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	1.43E-07	25	No consistent range - value from most recent review chosen (Montgomery 2007)								5.57E-01	1.722																
													0.0297	0.0297																
													10.435	10.435																
													0.0249	0.0249																
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	7.58E-02	25	No consistent range - value from most recent review chosen (Montgomery 2007)		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
						Geomean	No data	Insert Values		No data	Insert Values	25	3.00E+00	3.00E+00	25	No data	Insert Values		2.85E-01	2.85E-01	24	Not Reviewed	Insert Values		No data	Insert Values		No data	Insert Values	
													3.00E+00	3.00E+00	25				3.00E+00	3.00E+00	25									
													2.85E-01	2.85E-01	24				5.10E-04	5.10E-04	25									
													2.20E-02	2.20E-02	25															
													2.00E-02	2.00E-02	25															
													4.00E-02	4.00E-02	25															
													1.96	1.96E+00	25															
													0.0005	5.00E-04	25															
													0.00051	5.10E-04	25															
													0.00049	4.90E-04	25															
													0.0092	9.20E-03	25															
													0.0249	2.49E-02	25															
													0.0004	4.00E-04	25															
													0.00042	4.20E-04	25															
Chemical Boiling Point (ambient pressure)	K	n/a	6.59E+02	n/a	Median value chosen as central value from consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	No data	Insert Values	n/a	Insert Values	n/a	Insert Values	n/a	386	659.15	n/a	6.59E+02	n/a	Not Reviewed	Insert Values	n/a	659	659.00	n/a	No data	Insert Values	n/a	No data	Insert Values	n/a
Chemical Melting Point (ambient pressure)	K	n/a	2.48E+02	n/a	Three identical values from consistent range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	No data	Insert Values	n/a	248.15	248.15	n/a	-25	248.15	n/a	-25	248.15	n/a	Not Reviewed	Insert Values	n/a	No data	No data	n/a	No data	Insert Values	n/a	No data	Insert Values	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	8.04E+00	n/a	Median value chosen as central value from consistent range		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
						Average	No data	Insert Values	n/a	No data	No data	n/a	9.2	9.20	n/a	No data	8.17	8.17	Not Reviewed	Insert Values	n/a	No data	Insert Values	n/a	No data	Insert Values	n/a	No data	Insert Values	n/a
													9.2	9.20	n/a															
													8.06	8.06	n/a															
													8.29	8.29	n/a															
													8.71	8.71	n/a															
													4.6	4.60	n/a															
													9.87	9.87	n/a															
													5.22	5.22	n/a															
													7.9	7.90	n/a															
													8.06	8.06	n/a															
Molar Volume (Le Bas method)	cm3 mol <sup>-1</sup>	n/a	5.25E+02	n/a	Single Value								cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)															
						Average	n/a	n/a	n/a	n/a	n/a	n/a	524.8	524.80	n/a															
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	69804.94482	6.98E+04	n/a	Normal Boiling Point calculated value adopted								KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>																
						Average	n/a	n/a	n/a	No data	Insert Values		No data	Not reviewed	Insert Values															
Chemical Critical Point temperature (ambient pressure)	K	807.0964977	807	n/a	calculated value adopted								°C	K	Ref. Temp (C)															
						Average	n/a	n/a	n/a	840	840.00	n/a	n/a	n/a	n/a	#VALUE!	n/a	n/a	n/a	n/a	n/a									
Critical Pressure	atm	11.46719494	11.467	n/a	calculated value adopted								Bar	Atmosph	Ref. Temp (C)															
						Average	n/a	n/a	n/a	10.8	10.65877128	n/a	n/a	n/a	n/a	1.07E+01	?	n/a	n/a	n/a	n/a									

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	4.96E-12	10	Estimated from parameters above using Clapron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	9.74E-05	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	3.24E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	2.44E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	4.87	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Hexachloroethane	CAS Number:	67-72-1	Assessor A: Date	A Fellows - Ecologia 15.04.09	Assessor B: Date	J Brown - DTS Ra 16.04.09	Final review: Date	Panel/SF 28/08/2009
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	Oral	Dermal	Inhalation	Justification
Apply TDloral to exposure routes?	Yes	Yes	Yes	Group C carcinogen (IRIS), Insufficient evidence to be a human carcinogen - TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No	
Apply TDlinh to exposure routes?	No	No	No	Group C carcinogen (IRIS), Insufficient evidence to be a human carcinogen. Insufficient data to allow formulation of inhalation TDI. TDloral applied to inhalation exposure routes.
Apply IDinh to exposure routes?	No	No	No	

TDI oral	Recommended TDloral	Initial Units	CLEA Units	Justification
	1	mg/kg/day	ug.kg-1.d-1	most conservative value (USEPA and IRIS)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Units	Units	Confidence	Basis	Value	Units	UF	UF description	Study type	
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Sep-97	06/04/2009	MRL intermediate	0.01	mg/kg/day		10	no data	NOAEL	1	mg/kg/day	100	10 for extrapolation from animals to humans, 10 for inter human variability	rats
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Sep-97	06/04/2009	MRL acute	1	mg/kg/day		1000	no data	NOAEL	100	mg/kg/day	100	10 for extrapolation form animals to humans, 10 for human variability	rabbits
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Aug-06	06/04/2009	RFD	0.001	mg/kg/day		1	no data	no data	no data	no data	no data	no data	no data
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/01/1991	06/04/2009	RFD	0.001	mg/kg/day		1	Medium	NOEL	1	mg/kg/day	1000	10 to account for interspecies extrapolation, 10 for the range of sensitivity within the human population to xenobiotics and 10 for the use of a subchronic study.	rats
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	1999	14.04.09	TDI	0.0047	mg/kg/day		4.7		LOAEL	0.0047	mg/kg/day	10000	10 for animals to humans, 10 for human variability, 10 for non-chronic study and 10 for LOAEL	Sub-chronic oral

TDI inhal	Recommended TDlinhal	Initial Units	CLEA Units	Justification
	n/a	n/a	ug.kg-1.d-1	Current studies undertaken considered insufficient for derivation of TDI Inhalation. Using Oral Extrapolation.

Organisation	Last Updated	Date Web Checked	Health criteria type	Value	Units	Units	Confidence rating	Basis	Value	Units	UF	UF description	Study type	
International Agency for Research on Cancer (IARC)	1999	14.04.09	TDI	10	mg/m3		no data	LOAEL	10	mg/m3	no data	no data	Acute - Short term repeated dose	
International Programme on Chemical Safety (IPCS)	2004	14/04/2009	MAK - Maximum Workplace Concentration	9.8	mg/m3		2.8	no data	no data	9.8	mg/m3	no data	no data	Animal Study (rat)
Dutch National Institute for Public Health	N/A	14/04/2009	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	N/A	
Health Canada Toicological Values	Jun-05	06.04.09	no data	no data	no data	no data	no data	LOEC	465	mg/m3	no data	no data	female rats	
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	Sep-97	14.04.09	MRL intermediate	6	ppm		no data	NOAEL	48	ppm	30	10 for human variability, 3 for animal human extrapolation	Intermediate - Animal Study	
US Agency for Toxic Substances and Disease Registry (ATDSR) Toxicological Profiles and Minimal Risk levels	Sep-97	14.04.09	MRL acute	6	ppm		no data	NOAEL	48	ppm	30	10 for human variability, 3 for animal human extrapolation. Converted for humans by 48 ppm (0.22 m3/day/0.204kg) / 20 m3/day/70kg = 181 ppm	Acute - Animal Study	

Hexachloroethane
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<b>TDI oral</b>				
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Organisation	Description	Target organ/Critical Effect	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Groups of 10 male and 10 female rats fed HCE in diet for 16 weeks	liver and kidney weight increased	ATSDR, Toxicological Profile For Hexachloroethane, 1997	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Groups of 5 male New Zealand rabbits treated by gavage for 12 days.	liver degeneration and necrosis	ATSDR, Toxicological Profile For Hexachloroethane, 1997	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf</a>
USEPA Health Advisors	no data	no data	EPA, 2006 Edition of the Drinking Water Standards and Health Advisories, 2006	<a href="http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf">http://www.epa.gov/waterscience/criteria/drinking/dwstandards.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Groups of 10 male and 10 female rats fed HCE in diet for 16 weeks	liver and kidney weight increased	IRIS online database, last updated in 2003	<a href="http://www.epa.gov/NCEA/iris/subst/0167.htm#carc">http://www.epa.gov/NCEA/iris/subst/0167.htm#carc</a>
Toxicology Data Network (Toxnet)	Subchronic rat studies. In subchronic studies kidney degeneration at 15 and 62 mg/kg bw/day and increased kidney weights at 62 mg/kg were seen. Signs of kidney toxicity were seen at 47 mg/kg bw/day.	Kidneys	Nord Vol:15 (1999) pp 269-83	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~VYlc6H:5">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?./temp/~VYlc6H:5</a>

<b>TDI inhal</b>				
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Organisation	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)	In humans, exposure by inhalation to hexachloroethane (10-20 mg/m3) produced mild irritation of the skin and mucous membrane.	Skin	IARC Monographs on the evaluation of the carcinogenic risk of chemicals to humans Vol:73 (1999) pp 295-306	<a href="http://www.inchem.org/documents/iarc/vol73/73-10.html">http://www.inchem.org/documents/iarc/vol73/73-10.html</a>
International Programme on Chemical Safety (IPCS)	Occupational Exposure Limit (DFG 2004).	The substance may have effects on the liver and kidneys. Exposure at far above the OEL may have effects on the central nervous system, inducing tremors and ataxia.	International Chemical Safety Cards	<a href="http://www.inchem.org/documents/icsc/icsc/eics0051.htm">http://www.inchem.org/documents/icsc/icsc/eics0051.htm</a>
Dutch National Institute for Public Health	N/A	N/A	N/A	N/A
Health Canada Toxicological Values	LOEC for development toxicity. LOEC for short term repeated dose toxicity = 2517mg/m3 (different study)		Health Canada, State of the Science Report for a Screening Health Assessment – Hexachloroethane, 2005	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/hexachloroethane/hexachloroethane-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/contaminants/hexachloroethane/hexachloroethane-eng.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Groups of 25 male and female rats subjected to 0, 15, 48 and 260 ppm for 6 hrs/day, 5 days/week for 6 weeks.	Reduced body weight, eye irritation, tremors and reduced infection resistance.	ATSDR, Toxicological Profile For Hexachloroethane, 1997	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Groups of 22 pregnant rats exposed to vapours for 6 hrs day on gestation days 6-16.	Reduced body weight, eye irritation, tremors and reduced infection resistance.	ATSDR, Toxicological Profile For Hexachloroethane, 1997	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp97.pdf</a>



Hexachloroethane
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ID oral				
Organisation	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)	no data	After short-term exposure, hexachloroethane caused renal toxicity in male rats and hepatocellular necrosis in both male and female rats.	International Chemical Safety Cards	<a href="http://www.inchem.org/documents/icsc/icsc/eics0051.htm">http://www.inchem.org/documents/icsc/icsc/eics0051.htm</a>
USEPA Integrated Risk Information System (IRIS)		Tumor Type: Hepatocellular Carcinomas	IRIS online database. Last updated in 2003.	<a href="http://www.epa.gov/ncea/iris/subst/0167.htm">http://www.epa.gov/ncea/iris/subst/0167.htm</a>

ID inhal				
Organisation	Description	Response	Reference	Web link
International Agency for Research on Cancer (IARC)	no data	After short-term exposure, hexachloroethane caused renal toxicity in male rats and hepatocellular necrosis in both male and female rats.	International Chemical Safety Cards	<a href="http://www.inchem.org/documents/icsc/icsc/eics0051.htm">http://www.inchem.org/documents/icsc/icsc/eics0051.htm</a>
USEPA Integrated Risk Information System (IRIS)		Tumor Type: Hepatocellular Carcinomas	IRIS online database. Last updated in 2003.	<a href="http://www.epa.gov/ncea/iris/subst/0167.htm">http://www.epa.gov/ncea/iris/subst/0167.htm</a>

<b>Hexachloroethane</b>	CAS 67-72-1	Assessor A:	J. Brown - DTS Raeburn	Assessor B:	A. Fellows - Ecologia	Final Review	Panel/SF
		Date	14.04.09	Date	16.04.09	Date	28.08.09

MDI			Recommended MDI <sub>oral</sub>	Units	Justification: From Health Canada. Back calculated for CLEA adult.		
			14.02	ug day-1			
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Health Canada Toxicological Reference Values	June 28th 2005	drinking water, food and beverages, soil.	14.02	ug/day	adult age group based on data from Canadian surveys of drinking water, food and beverages. Back-calculated for CLEA adult	Health Canada, State of the Science Report for a Screening Health Assessment – Hexachloroethane, 2005	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>
Other					Hexachloroethane on List 1 of Groundwater regulations 1998	Department of the Environment, Transport and the Regions, Guidance on the Groundwater Regulations 1998, 2001	<a href="http://www.defra.gov.uk/environment/water/ground/pdf/groundwater-guidance.pdf">http://www.defra.gov.uk/environment/water/ground/pdf/groundwater-guidance.pdf</a>

MDI			Recommended MDI <sub>inh</sub>	Units	Justification: Health Canada values for indoor and outdoor air, back calculated for CLEA respiration rate.		
			8.64E+01	ug day-1			
Organisation	Date	Media	Value	Units	Description	Reference	Web link
International Programme on Chemical Safety (IPCS)	Dec-08	air	0.15	ppm	odour threshold	<a href="http://www.who.int/ipcs/publications/icsc/comp_guide.pdf">http://www.who.int/ipcs/publications/icsc/comp_guide.pdf</a>	<a href="http://www.who.int/ipcs/en">www.who.int/ipcs/en</a>
Health Canada Toxicological Reference Values	June 28th 2005	indoor and outdoor air	86.4	µg/day	estimated total intake, based on data from Canadian surveys of indoor and outdoor air concentrations (1.0002 ug/kg/day), back calculated to reflect CLEA adult	Health Canada, State of the Science Report for a Screening Health Assessment – Hexachloroethane, 2005	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>
Other	15-Apr-09	Ambient air	1	ug/day	US study of 930 samples with a median concentration of 9.1 ppt	Howard et al 1990, Handbook of Env Fate and Exposure data for Organic chemicals , Volume 2	



Isopropylbenzene	CAS Number:	98-82-8	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	Simon Tempest (ERM)	Final review:	Panel/SF
	Date	19/05/2009	Date	20/05/2009	Date	28/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDI <sub>oral</sub> to exposure routes?	Yes	Yes	No	Yes	Unclassified by IARC, USEPA Group D not classifiable as to human carcinogenicity - TDI <sub>oral</sub> applied to oral and dermal routes
Apply ID <sub>oral</sub> to exposure routes?	No	No	No		
Apply TDI <sub>inh</sub> to exposure routes?	No	No	Yes		Unclassified by IARC, USEPA Group D not classifiable as to human carcinogenicity- TDI <sub>inh</sub> applied to inhalation routes
Apply ID <sub>inh</sub> to exposure routes?	No	No	No		

TDI oral	Recommended TDI <sub>oral</sub>	Units	Justification
	100	µg/kg.bw/day	CICADs, IRIS, USEPA Region 9, RAIS, Texas provide consistent value

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	unknown	18/05/2009	NOAEL	154	mg/kg/bw/day	154,000		NOAEL	154	mg/kg/bw/day		0 Rats are reported to be one of the most sensitive animal to cumene. Toxicokinetics not reportedly qualitatively different between humans and animals.	oral gavage study of rats
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://incem.org/pages/cicads.html">http://incem.org/pages/cicads.html</a>	unknown	18/05/2009	Guidance Value	0.1	mg/kg/bw/day	100		NOAEL	110	mg/kg/bw/day	1000	10 - interindividual 10 - interspecies 10 -0.5 - sub chronic to chronic 10 -0.5 - lack of full scale multi-generation reproductive study	oral (gavage) study of rats
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/08/1997	19/05/2009	RfD	0.1	mg/kg/bw/day	100	Low	NOAEL	110	mg/kg/bw/day	1000	10 - interspecies variation 10 - intraspecies variation 3 - sub chronic to chronic 3 - database deficiencies (lack of reproductive information)	Rat
USEPA Region 9 Preliminary Remediation Goals	<a href="http://www.epa.gov/region09/superfund/prg/">http://www.epa.gov/region09/superfund/prg/</a>	12/05/2009	19/05/2009	RfD	0.1	mg/kg/bw/day	100		unknown					unknown
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trppcls.html</a>	26/03/2009	19/05/2009	RfD	0.1	mg/kg/bw/day	100		unknown					unknown
The Risk Assessment Information System (RAIS)	<a href="http://rais.ornl.gov/">http://rais.ornl.gov/</a>	17/08/2005	19/05/2009	RfD	0.1	mg/kg/bw/day	100	Low	NOAEL/LOAEL			1000	unknown	Rat

## Isopropylbenzene

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
European Chemicals Bureau (ECB)	6 month study of rats for cumene administered in olive oil by gavage.	Depression of CNS and increases in liver, kidney and dermal gland weight.	European Commission, Joint Research Centre, August 1999. Cumene, Summary Risk Assessment Report. (Preface of report states "summary report should preferably not be used for citation purposes")	<a href="http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/RISK_ASSESSMENT/SUMMARY/cumenesum007.pdf">http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/RISK_ASSESSMENT/SUMMARY/cumenesum007.pdf</a>
IPCS concise International Chemical Assessment Documents (CICADs)	increased average kidney weight in rats following sub-chronic (139/194 days) oral exposure in study by Wolf et al 1956.	Kidneys. Increase in organ weight (most notably the kidney).	IPCS INCHEM, 1999. Concise International Chemical Assessment Document 18. Cumene.	<a href="http://incchem.org/documents/cicads/cicads/cicad18.htm">http://incchem.org/documents/cicads/cicads/cicad18.htm</a>
USEPA Integrated Risk Information System (IRIS)	194 day rat oral gavage study by Wolf et al 1956.	Increased average kidney weight in female rats	USEPA. Integrated Risk Information System. Cumene (CAS 98-82-8). Accessed 19th May 2009.	<a href="http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nmbr=0306">http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nmbr=0306</a>
USEPA Region 9 Preliminary Remediation Goals	RfD sourced from IRIS	unknown	USEPA Region 9. Preliminary Remediation Goals, Screening Levels for Contaminants. Accessed 19th May 2009.	<a href="http://www.epa.gov/region09/superfund/prg/pdf/indsoil_sl_table_run_APRIL2009.pdf">http://www.epa.gov/region09/superfund/prg/pdf/indsoil_sl_table_run_APRIL2009.pdf</a>
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	RfD sourced from IRIS	unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 19th May 2009.	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html</a>
The Risk Assessment Information System (RAIS)	study by Wolf et al 1956 referenced by IRIS.	Kidney / Increased average kidney weight in female rats	Risk Assessment Information System (RAIS). Accessed 19th May 2009.	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select">http://rais.ornl.gov/cgi-bin/tox/TOX_select</a>

Isopropylbenzene		CAS Number:	98-82-8	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	Simon Tempest (ERM)	Final review:	Panel/SF					
		Date	19/05/2009	Date	20/05/2009	Date	28/08/2009							
TDI inhal				Recommended TDIinhal	Units	Justification								
				114.3	µg/kg.bw/day	CICAD (NOAEL/LOAEL), IRIS, USEPA Region 9, RAIS, Texas provide consistent value. CICAD NOAEL not considered as NOAEL has been demonstrated within the same source at concentrations greater than this. USEPA Acute criteria not considered appropriate for assessing chronic risks.								
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg.1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
European Chemicals Bureau (ECB)	<a href="http://ecb.irc.it/">http://ecb.irc.it/</a>	unknown	18/05/2009	NOAEL	490	mg/m3	140000		NOAEL	490	mg/m3		0 Rats are reported to be one of the most sensitive animal to cumene. Toxicokinetics not reportedly qualitatively different between humans and animals.	rats
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	unknown	18/05/2009	Guidance Value	0.4	mg/m3	114.3		NOAEL but also regarded as a potential LOAEL (adjusted for continuous exposure)	436	mg/m3	1000	10 - interindividual 10 - sub chronic to chronic 10 -0.5 - interspecies 10 -0.5 - database deficiencies (lack of full scale multi-generation reproductive study)	rats
IPCS concise International Chemical Assessment Documents (CICADs)	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>	unknown	18/05/2009	Guidance Value	0.09	mg/m3	25.7		NOAEL (adjusted for continuous exposure)	88	mg/m3	1000	10 - interindividual 10 - sub chronic to chronic 10 -0.5 - interspecies 10 -0.5 - database deficiencies (lack of full scale multi-generation reproductive study)	rats
USEPA Acute Guideline Levels (AEGLS)	<a href="http://epa.gov/oppt/aegl/pubs/chemlist.htm">http://epa.gov/oppt/aegl/pubs/chemlist.htm</a>	13/02/2009	19/05/2009	Acute Exposure Guideline Value - AEG1 (non disabling 8 hour duration)	250	mg/m3	71428		Value painful to eyes	300	ppm		6 2 - cause effect within scope of AEG1 i.e. mild eye and respiratory irritation. 3- intraspecies variability	Human & rat data
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	27/04/2009	19/05/2009											
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/08/1997	19/05/2009	RfC	0.4	mg/m3	114.3	medium	NOAEL	435	mg/m3	1000	10 - sub chronic to chronic 10 - intraspecies variation 3 - interspecies variation 3 - database deficiencies (lack of reproductive studies)	Rat
USEPA Region 9 Preliminary Remediation Goals	<a href="http://www.epa.gov/region09/superfund/prg/">http://www.epa.gov/region09/superfund/prg/</a>	12/05/2009	19/05/2009	RfC	0.4	mg/m3	114.3		unknown					unknown
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html</a>	26/03/2009	19/05/2009	RfC	0.4	mg/m3	114.3		unknown					unknown
The Risk Assessment Information System (RAIS)	<a href="http://rais.ornl.gov/">http://rais.ornl.gov/</a>	17/08/2005	19/05/2009	RfC	0.4	mg/m3	114.3	medium	NOAEL/LOAEL			1000	unknown	Rat

## Isopropylbenzene

TDI inhal

Organisation	Description	Response	Reference	Web link
European Chemicals Bureau (ECB)	90 day exposure study of rats exposed to 500 and 1200ppm cumene	Depression of CNS and increases in liver, kidney and dermal gland weight.	European Commission, Joint Research Centre, August 1999. Cumene, Summary Risk Assessment Report. (Preface of report states "summary report should preferably not be used for citation purposes")	<a href="http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/RISK_ASSESSMENT/SUMMARY/cumenesum007.pdf">http://ecb.jrc.ec.europa.eu/documents/Existing-Chemicals/RISK_ASSESSMENT/SUMMARY/cumenesum007.pdf</a>
IPCS concise International Chemical Assessment Documents (CICADs)	3 month sub chronic inhalation study by Cushman et al 1995.	increased kidney and adrenal weights and central nervous system, haematological, and clinical biochemical alterations, which were observed in rats.	IPCS INCHEM, 1999. Concise International Chemical Assessment Document 18. Cumene.	<a href="http://inchem.org/documents/cicads/cicads/cicad18.htm">http://inchem.org/documents/cicads/cicads/cicad18.htm</a>
IPCS concise International Chemical Assessment Documents (CICADs)	3 month sub chronic inhalation study by Cushman et al 1995.	Increased kidney and adrenal weights and central nervous system, haematological, and clinical biochemical alterations, which were observed in rats.	IPCS INCHEM, 1999. Concise International Chemical Assessment Document 18. Cumene.	<a href="http://inchem.org/documents/cicads/cicads/cicad18.htm">http://inchem.org/documents/cicads/cicads/cicad18.htm</a>
USEPA Acute Guideline Levels (AEGLs)	volunteers willingly tolerated exposure to 49-146 ppm cumene for an 8-hour period with two 30-minute breaks & several rat studies (a single or multiple exposures for 6 hours to 100 ppm caused no toxic effects)	Mild eye and respiratory irritation in humans	USEPA. Acute Exposure Guidelines (AEGLs) for Cumene (CAS 98-82-8). Interim 1- 8/2007.	<a href="http://epa.gov/oppt/aegl/pubs/cumene_tsd_interimversion1_8_28_07.pdf">http://epa.gov/oppt/aegl/pubs/cumene_tsd_interimversion1_8_28_07.pdf</a>
USEPA Health Advisors				
USEPA Integrated Risk Information System (IRIS)	13 week inhalation study of rats by Cushman et al 1995.	Increased kidney weights in female rats and adrenal weights in male and female rats	USEPA. Integrated Risk Information System. Cumene (CAS 98-82-8). Accessed 19th May 2009.	<a href="http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nbr=0306">http://cfpub.epa.gov/ncea/iris/index.cfm?fuseaction=iris.showQuickView&amp;substance_nbr=0306</a>
USEPA Region 9 Preliminary Remediation Goals	RfC sourced from IRIS	unknown	USEPA Region 9. Preliminary Remediation Goals, Screening Levels for Contaminants. Accessed 19th May 2009.	<a href="http://www.epa.gov/region09/superfund/prg/pdf/indsoil_sl_table_run_APR_IL2009.pdf">http://www.epa.gov/region09/superfund/prg/pdf/indsoil_sl_table_run_APR_IL2009.pdf</a>
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	RfC sourced from IRIS	unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 19th May 2009	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppcls.html</a>
The Risk Assessment Information System (RAIS)	study by Cushman et al 1995 referenced by IRIS.	Kidney / Increased kidney weights in female rats and adrenal weights in male and female rats	Risk Assessment Information System (RAIS). Accessed 19th May 2009.	<a href="http://rais.ornl.gov/cgi-bin/tox/TOX_select">http://rais.ornl.gov/cgi-bin/tox/TOX_select</a>

Isopropylbenzene	CAS 98-82-8	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	Simon Tempest (ERM)	Final review:	Panel/SF
		Date	19/05/2009	Date	01/06/2009	Date	28/08/2009

MDI	Recommended MDI <sub>oral</sub>	Units	Justification: The available qualitative information (ECB) indicates that background exposure via food and water is considered to be negligible in comparison to HCV. HCV is equivalent to drinking water concentration of 3500µg/L based on a 70kg adult consuming 2L/day.
	0	µg day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
European Chemicals Bureau (ECB)	01/06/2009		Negligible	µg.day <sup>-1</sup>	The report states that "model predictions suggest that by far the greater amount of human exposure via the environment will be from the air, contributing some 97% of the intake".	European Commission, Joint Research Centre, August 1999. Cumene, Summary Risk Assessment Report. (Preface of report states "summary report should preferably not be used for citation purposes")	<a href="http://ecb.irc.it/">http://ecb.irc.it/</a>

MDI	Recommended MDI <sub>inh</sub>	Units	Justification: Based on reported ambient cumene concentration reported in IPCS CICADs
	294	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
European Chemicals Bureau (ECB)	01/06/2009	Air	1	ug/day	Based on regional exposure level of 1.45e-5 mg/kg/bw/day from the EUSES model	European Commission, Joint Research Centre, August 1999. Cumene, Summary Risk Assessment Report. (Preface of report states "summary report should preferably not be used for citation purposes")	<a href="http://ecb.irc.it/">http://ecb.irc.it/</a>
IPCS Concise International Chemical Assessment Documents (CICADs)	01/06/2009	Air	294	ug/day	Based on reported ambient cumene concentration of 0.0147mg/m <sup>3</sup> .	IPCS INCHEM, 1999. Concise International Chemical Assessment Document 18. Cumene.	<a href="http://inchem.org/pages/cicads.html">http://inchem.org/pages/cicads.html</a>

Substance:	<b>Iso-propylbenzene</b>	CAS Number:	98-82-8	Assessor A:	Simon Clennell-Jones (WSP)	Assessor B:	Alan Wilson (ERM)	Final Review:	Panel/SF
Chemical Formula:	C <sub>9</sub> H <sub>12</sub>	Phase at Ambient Temperature:	Liquid	Date:	20.04.2009	Date:	19.05.2009	Date:	28.08.2009

<http://srdata.nist.gov/solubility/>

<http://webbook.nist.gov/chemistry/>

<http://cs3-hq.oecd.org/scripts/hpv/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A			B			C			D			E			F			G			H		
							HOWARD, 1990			LIDE, 2008			MACKAY et al, 2006			MERCX, 2006			MONTGOMERY, 2007			MONTGOMERY, 1997			NIST, 2005			OECD, 2000		
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																														
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	120.191	n/a	Consistent value		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
							Average	Insert Values	n/a	120.191	120.191	n/a	120.191	120.191	n/a	120.19	120.19	n/a	120.19	120.19	n/a	120.19	120.19	n/a	120.1916	120.1916	n/a	120.2	120.2	n/a
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	1.47E+03	25	No consistent values, most recent source		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
							Geomean	Insert Values	25	1.466	1.47E+03	25	1469	1469	25	n/a	n/a	n/a	0.00558	5.65E+02	25	0.087	1.15E+03	25	0.068	1.48E+03	25	0.068	1.48E+03	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	56.00	25	Median value from consistent range		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
							Geomean	Insert Values	n/a	0.056	5.60E+01	25	73	7.30E+01	25	48.3	4.83E+01	n/a	48.3	4.83E+01	n/a	53	5.30E+01	25	50	5.00E+01	25	50	5.00E+01	25
Chemical Boiling Point (ambient pressure)	K	n/a	425.55	n/a	Central Value From Consistent Range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							Average	Insert Values	n/a	152.41	4.26E+02	n/a	152.41	4.26E+02	n/a	152	4.2515	n/a	152.4	4.2515	n/a	425	4.25E+02	n/a	425	4.25E+02	n/a	152.39	4.254	n/a
Chemical Melting Point (ambient pressure)	K	n/a	177.13	n/a	Central Value From Consistent Range		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							Average	Insert Values	n/a	-96.02	1.77E+02	n/a	-96.02	1.77E+02	n/a	-96	1.7715	n/a	-96	1.7715	n/a	177	1.77E+02	n/a	177	1.77E+02	n/a	177	1.77E+02	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	3.65	n/a	Central Value From Consistent Range		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
							Average	Insert Values	n/a	3.66	3.65E+00	n/a	3.43	3.43	n/a	3.63	3.63	n/a	3.63	3.66	n/a	3.66	3.66	n/a	3.66	3.66	n/a	3.66	3.66	n/a
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	162.6	n/a	single value		n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
							Average						162.6	162.60	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	37021.76274	37,022	n/a	Normal Boiling Point		n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
							Average			37.167	37167	n/a	37.53	37530	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Chemical Critical Point temperature (ambient pressure)	K	634.1308585	634.1	n/a	Calculated Value		n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
							Average			631	6.31E+02	n/a	n/a	n/a	n/a	Insert Values	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Critical Pressure	atm	32.33388501	32.33	n/a	Calculated Value		n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							Average			32.09	3.17E+01	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

**Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)**

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	0.237	10	Estimated from parameters above using Clapron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	266.990	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	6.49E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	4.87E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	3.06	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

<b>Isopropyltoluene</b>	<b>CAS Number:</b>	<b>99-87-6</b>	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panerl/SF
			Date	15/04/2009	Date	07/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	NR	Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		

<b>TDI oral</b>	<b>Recommended TDloral</b>	<b>Units</b>	<b>Justification</b>
	-	ug.kg-1.d-1	Insufficient data with sufficient detail on derivation to derive TDI

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Unknown	15/04/2009	Oral reference dose	1.00E-01	mg.kg-1.day-1	100	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/mediation/rrr.htm">http://www.tceq.state.tx.us/mediation/rrr.htm</a>	Mar-06	05/06/2009	Oral reference dose	1.00E-01	mg.kg day <sup>-1</sup>	100	Unknown	Unknown	Unknown

<b>TDI inhal</b>	<b>Recommended TDlinhal</b>	<b>Units</b>	<b>Justification</b>
	-	ug.kg-1.d-1	Insufficient data with sufficient detail on derivation to derive TDI

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/mediation/rrr.htm">http://www.tceq.state.tx.us/mediation/rrr.htm</a>	Mar-06	05/06/2009	Inhalation reference dose	8.60E-02	mg.kg day <sup>-1</sup>	86	Unknown	Unknown	Unknown

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**Isopropyltoluene**


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TDI oral								
Organisation	Units	UF	UF description	Study type	Description	Target organ/Critical Effect	Reference	Web link
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	ATSDR Health Consultation for DETCO Industries, Arkansas, April 4 2005 RfD is quoted in this report (page 5) but unable to find the study reference etc.	<a href="http://www.atsdr.cdc.gov/HAC/pha/DetcoIndApr05/DetcoSurfaceWaterHCfinal040405.pdf">http://www.atsdr.cdc.gov/HAC/pha/DetcoIndApr05/DetcoSurfaceWaterHCfinal040405.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>
TDI inhal								
Organisation	Units	UF	UF description	Study type	Description	Response	Reference	Web link
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

<b>Isopropyltoluene</b>	CAS 99-87-6	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panel/SF
		Date	15/04/2009	Date	06/05/2009	Date	28/08/2009

Organisation	Date	Media	Value	Units	Description	Reference	Web link
<b>MDI</b>			<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, likely to be negligible.		
			0	ug day <sup>-1</sup>			
<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Only available data (TOXNET). Converted assuming an adult breathes 20m <sup>3</sup> /day.		
			880	ug day <sup>-1</sup>			
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Toxicological Data Network (TOXNET)	06/04/2009	Suburban air	880	ug.day <sup>-1</sup>	0.005-0.008 ppm recorded in suburban air in Longbeach, CA, US. This is equivalent to 0.027 to 0.044 mg/m <sup>3</sup> , which can be converted to 880µg/day assuming an adult breathes 20 m <sup>3</sup> /day.	Neligan RE et al; The Gas Chromatographic Determination of Aromatic Hydrocarbons in the Atmosphere. ACS Natl Mtg p. 118-21 (1965) (2) Brown SK et al; Indoor Air 4: 123-34 (1994) (3) Helmig D, Arey J; Sci Total Environ 112: 233-50 (1992)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>



Methyl tert-butyl ether	CAS Number: 1634-04-4	Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF
		Date 01/03/2009	Date 27/04/2009	date: 26/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Consensus that MTBE not genotoxic. HCV based on threshold effects. TDloral applied to oral and dermal routes
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	300	ug.kg-1.d-1	Consensus of two literature values identified (RIVM and ATSDR)

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	2002	27/04/2009	Various repeated toxicity animal studies and occupational human studies available but no TDI derived.					NOAEL	300	mg/kg		Reliable data	Repeated dose toxicity
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1998	27/04/2009	No recommended HCV but several animal studies					NOAEL	90	mg.kg bw-1.d-1			Short-term repeated dose study
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2005	27/04/2009						NOAEL	100	mg.kg bw-1.d-1			Longer term oral dose study
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2004	25/03/2009	Max. Permissible Risk	0.3	mg. kg bw-1.d-1	300		LOAEL	a) 300 b) 200	mg.kg bw-1.d-1 mg.kg bw-1.d-1	1000		Subchronic studies
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	2006	25/03/2009											
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	1996	25/03/2009	Oral MRL	0.3	mg. kg bw-1.d-1	300		LOAEL	100	mg.kg bw-1.d-1			Intermediate duration Oral study
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Dec-97	25/03/2009	No low dose values available, but animal studies presented					LOAEL	300	mg.kg bw-1.d-1			
Entrez PubMed	<a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">http://www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>	Current	26/03/2009	More info available within full document										Subchronic

**Methyl tert-butyl ether**

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
European Chemicals Bureau (ECB)	Oral NOAEL of 300 mg/kg based on a) 90 day study of Sprague-Dawley rats b) Male rat study	a) Elevated AST with weight increase at 900 mg/kg b) Slight morphological liver abnormalities at 200 mg/kg	a) Robinson M, Bruner RH & Olson GR (1990). Fourteen- and ninety-day oral toxicity studies of methyl tertiary-butyl ether in Sprague-Dawley rats. Journal of the American College of Toxicology, 9, 525-540. b) Zhou W & Ye S (1999). Subchronic Oral Methyl Ter	<a href="http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf">http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf</a>
IPCS Environmental Health Criteria (EHC) Monographs	In a 28-day oral study, Sprague-Dawley rats (10/sex/group) were administered 0, 90, 440 or 1750 mg undiluted MTBE (purity not specified)/kg bw daily by gavage for a total of 20 h (IITRI, 1992).	Increased kidney weights	IITRI (1992) 28-day oral (gavage) toxicity of methyl tert-butyl ether (MTBE) in rats (Project No. L08100). Chicago, Illinois, Illinois Institute of Technology Research, 48 pp.	<a href="http://incchem.org/documents/ehc/ehc/ehc206.htm#SubSectionNumber:7.4.1">http://incchem.org/documents/ehc/ehc/ehc206.htm#SubSectionNumber:7.4.1</a>
WHO Guidelines for drinking water Quality	In a 90 day study groups of 10 male and female rats were administered 0, 100,300, 900 or 1200 mg.kg bw-1. d-1 of MTBE in corn oil	Increase in relative kidney weight	Robinson M, Bruner RH, Olson GR (1990) Fourteen- and ninety-day oral toxicity studies of methyl tertiary-butyl ether in Sprague-Dawley rats. Journal of the American College of Toxicology, 9: 525–540.	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/MTBE200605.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/MTBE200605.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	a) 90 day oral by gavage study in rats  b) 90 day oral by gavage study in rats	a) Kidney and liver toxicity  b) Increased liver and kidney weight	TDI within ECB (2002) based on a) and b). ECB (2002). European Union Risk Assessment Report t-butyl methyl ether. European Chemicals Bureau, 3rd Priority list, volume 19; Office for Official Publications of the EC, Luxembourg. a) Robinson M, Bruner RH, Ol	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701039.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701039.pdf</a>
Health Canada Toxicological Values	Health Canada has determined that there exist too many uncertainties and limitations in the MTBE database to have confidence in a quantitative risk assessment for human health.		Guidelines for Canadian Drinking Water Quality: Guideline Technical Document. Methyl Tertiary-Butyl Ether (MTBE). Health Canada, Ottawa, Ontario, July 2006	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/water_eau/mtbe/mtbe-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/water_eau/mtbe/mtbe-eng.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	90 day study	Hepatic effects	Robinson M, Bruner RH, Olson GR (1990) Fourteen- and ninety-day oral toxicity studies of methyl tertiary-butyl ether in Sprague-Dawley rats. Journal of the American College of Toxicology, 9: 525–540.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp91.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp91.pdf</a>
USEPA Health Advisors	90 day oral exposure study in rats	Kidney effects	Robinson M, Bruner RH, Olson GR (1990) Fourteen- and ninety-day oral toxicity studies of methyl tertiary-butyl ether in Sprague-Dawley rats. Journal of the American College of Toxicology, 9: 525–540.	<a href="http://www.epa.gov/waterscience/criteria/drinking/mtbe.pdf">http://www.epa.gov/waterscience/criteria/drinking/mtbe.pdf</a>
Entrez PubMed	MTBE administered to rats at doses of 0,400,800 and 1600 mg. Kg bw-1.d-1.	Relative change in heart, liver, kidney, testes, thymus and prostate weight	Effects of subchronic methyl tert-butyl ether ether exposure on male Sprague-Dawley rats. Dong-Mei L, Yi G, Chun-Tao Y, Yu-Feng H, Xiao-Dong H. Toxicol Ind Health. 2009 Feb;25(1):15-23.	<a href="http://www.ncbi.nlm.nih.gov/pubmed/19318501?ordinalpos=2&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/19318501?ordinalpos=2&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>

Methyl tert-butyl ether	CAS Number: 1634-04-4	Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF
		Date 01/03/2009	Date 27/04/2009	date: 26/08/2009

TDI inhal	Recommended TDIinhal	Units	Justification
	722	ug.kg-1.d-1	General consistency amongst RIVM, ATSDR and IRIS values, most conservative value chosen (ATSDR). All available values based on same tox study. Conversion using ATSDR MRL; 0.7ppm x 3610µg.m-3.ppm-1 x 20m3.day-1 / 70kg).

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Committee on the Medical Effects of Air Pollutants (COMEAP)	<a href="http://www.advisorybodies.doh.gov.uk/comeap/index.htm">http://www.advisorybodies.doh.gov.uk/comeap/index.htm</a>	Sep-00	27/04/2009							3142	mg.m-3			Inhalation
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	2002	27/04/2009	Various repeated toxicity animal studies and occupational human studies available but no TDI derived.					NOAEL	300	mg.kg bw-1.d-1	Unknown		Inhalation. Repeat dose toxicity
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1998	27/04/2009						NOAEL	1440	mg.m-3			Mid length inhalation exposure study
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	2005	27/04/2009						NOAEL	210	mg. Kg bw-1.d-1			Neurotoxicity study inhalation
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2004	25/03/2009	TCA	2.6	mg.m-3	742		NOAEL	1440	mg.m-3		Uses correction factor for exposure duration and UF of 100 and rounding off	Subchronic inhalation
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	1996	27/04/2009	MRL (Conversion 1ppm=3.61mg/m³)	0.7	ppm (1ppm = 3.61mg/m³)	722		NOAEL	400 (1444)	ppm (mg/m³)	100		Intermediate Inhalation
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	01/09/1993	26/03/2009	Inhal RfC	3	mg.m-3	857		NOAEL	1453	mg.m-3	100	An uncertainty factor of 10 is applied to account for extrapolation to sensitive human subpopulations. An additional factor of 3 is used to account for interspecies extrapolation. A full 10-fold adjustment for interspecies extrapolation is not deemed necessary.	Chronic

ID oral	Recommended IDoral	Units	Justification
			Consensus that MTBE not genotoxic

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	2002	27/04/2009	MTBE is not a genotoxic substance		LOAEL	250	mg/kg bw-1.d-1	Not very high		
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	Sep-99	27/04/2009	The data indicate that methyl tert-butyl ether is not genotoxic							
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1998	27/04/2009	The weight of evidence indicates that MTBE is not genotoxic.							
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2004	27/04/2009	The weight of evidence indicates that MTBE is not genotoxic.							

## Methyl tert-butyl ether

TDI inhal
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Organisation	Description	Response	Reference	Web link
Committee on the Medical Effects of Air Pollutants (COMEAP)	Rat study	Motor activity affected	Health Effects Institute: The Potential Health Effects of Oxygenates added to Gasoline (1996).	<a href="http://www.advisorybodies.doh.gov.uk/comeap/pdfs/comeap-99-00.pdf">http://www.advisorybodies.doh.gov.uk/comeap/pdfs/comeap-99-00.pdf</a>
European Chemicals Bureau (ECB)	An inhalation NOAEC of 800 ppm has been used based on a) inhalation exposure in a 13 week rat study b) 2 year rat study	a) mild liver effects at 4000 ppm b) mild liver effects at 3000 ppm	a) Lington AW, Dodd DE, Ridlon SA, Douglas JF, Kneiss JJ & Andrews LS (1997). Evaluation of 13-week inhalation toxicity study on methyl t-butyl ether (MTBE) in Fischer 344 rats. Journal of Applied Toxicology, 17. b) Bird MG, Burleigh-Flayer HD, Chun JS, Dou	<a href="http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf">http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf</a>
IPCS Environmental Health Criteria (EHC) Monographs	An oncogenicity study was also carried out on CD-1 mice exposed to MTBE (99% pure) vapour in inhalation chambers (Burleigh-Flayer et al., 1992; Bird et al., 1997). Groups of 50 male and 50 female mice were exposed to target concentrations of 0, 1430, 10 7	Effects on the liver	Burleigh-Flayer HD, Chun JS, & Kintigh WJ (1992) Methyl tertiary butyl ether: vapor inhalation oncogenicity study in CD-1 mice (Laboratory project ID 91N0013A). Export, Pennsylvania, Bushy Run Research Center, 1068 pp (Report to the Methyl Tertiary Butyl	<a href="http://incem.org/documents/ehc/ehc/ehc206.htm#SubSectionNumber:7.4.2">http://incem.org/documents/ehc/ehc/ehc206.htm#SubSectionNumber:7.4.2</a>
WHO Guidelines for drinking water Quality	Daily exposure of male and female rats to MTBE at 2900 mg.m-3 for 13 weeks	Absolute but not relative decrease in brain weight	Miller MJ et al. (1997) Pharmacokinetics and disposition of methyl t-butyl ether in Fischer-344 rats. Journal of Applied Toxicology, 17(Suppl. 1): S3-S12.	<a href="http://www.who.int/water_sanitation_health/dwa/chemicals/MTBE200605.pdf">http://www.who.int/water_sanitation_health/dwa/chemicals/MTBE200605.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	28 day inhalation study of rat. Exposure of 6 hrs/day, 5 days/week	Increased liver and kidney weight	TCA from ECB (2002) based on Chun et al. 1993. ECB (2002). European Union Risk Assessment Report t-butyl methyl ether. European Chemicals Bureau, 3rd Priority list, volume 19; Office for Official Publications of the EC, Luxembourg.	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701039.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701039.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	24 month inhalation rat study. Exposure of 6 hr/day, 5 d/week.	Increased liver and kidney weight	RFC from IRIS 1996 based on Chun JS, Burleigh-Flayer HD, Kintigh WJ. 1992. Methyl tertiary butyl ether: Vapor inhalation oncogenicity study in Fischer 344 rats. Bushy Run Research Center, Export, PA. Project No. 91N0013B.	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp91.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp91.pdf</a>
USEPA Integrated Risk Information System (IRIS)	24 month inhalation rat study. Exposure of 6 hr/day, 5 d/week.	Increased absolute and relative liver and kidney weights and increased severity of spontaneous renal lesions (females), increased prostration (females), and swollen periocular tissue (males and females)	Chun, J.S., H.D. Burleigh-Flayer, and W.J. Kintigh. 1992. Methyl tertiary butyl ether: vapor inhalation oncogenicity study in Fischer 344 rats (unpublished material). Prepared for the MTBE Committee by Bushy Run Research Center, Union Carbide Chemicals.	<a href="http://www.epa.gov/ncea/iris/subst/0545.htm">http://www.epa.gov/ncea/iris/subst/0545.htm</a>

ID oral
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Organisation	Description	Response	Reference	Web link
European Chemicals Bureau (ECB)	Tumours have been reported in rats at doses $\leq$ 250 mg.kg-1			
International Agency for Research on Cancer (IARC)				
IPCS Environmental Health Criteria (EHC) Monographs				
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels				

Methyl tert-butyl ether	CAS Number: 1634-04-4	Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Jennifer Stothert, Entec UK Ltd	Final Review: Panel/SF
		Date 01/03/2009	Date 27/04/2009	date: 26/08/2009

ID inhal	Recommended IDInhal	Units	Justification
			Consensus that MTBE not genotoxic

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis	Study type
European Chemicals Bureau (ECB)	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>	2002	27/04/2009	MTBE is not a genotoxic substance			400	ppm		NOAEC	
International Agency for Research on Cancer (IARC)	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>	Sep-99	27/04/2009	The data indicate that methyl tert-butyl ether is not genotoxic							
IPCS Environmental Health Criteria (EHC) Monographs	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>	1998	27/04/2009	The weight of evidence indicates that MTBE is not genotoxic.							
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	2004	27/04/2009	The weight of evidence indicates that MTBE is not genotoxic.							

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**Methyl tert-butyl ether**

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Organisation	Description	Response	Reference	Web link
European Chemicals Bureau (ECB)	Tumours in rats and mice at doses $\geq$ 3,000 ppm after inhalation exposure			<a href="http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf">http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf</a>
International Agency for Research on Cancer (IARC)				
IPCS Environmental Health Criteria (EHC) Monographs				
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels				

MTBE	CAS 1634-04-4	Assessor A:	Cheryl Davies, Delta-Simons	Assessor B:	Sian Jones, Entec UK Ltd	Final Review:	Panel/SF
		Date	01/03/2009	Date	27/04/2009	Date	26/08/2009

MDI	Recommended MDI <sub>oral</sub>	Units	Justification: Based on data in UK Energy Institute report (Other). 94% of well fields sampled in UK had less than detection limit (typically 0.5µg/L). Average intake calculated assuming 0.5µg/L, converted assuming 2L/day consumed. Food intake assumed negligible.
	1	ug day <sup>-1</sup>	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Drinking Water Inspectorate	23/03/2009	Drinking water	5 to 10	ug l-1	Taste and odour threshold	<a href="http://www.dwi.gov.uk/consumer/consumer/mtbe.htm">http://www.dwi.gov.uk/consumer/consumer/mtbe.htm</a>	<a href="http://www.dwi.gov.uk/consumer/consumer/mtbe.htm">http://www.dwi.gov.uk/consumer/consumer/mtbe.htm</a>
Committee on the Medical Effects of Air Pollutants (COMEAP)	23/03/2009	Drinking water	15	ug l-1	From USEPA Drinking water Advisory odour detection levels 15 to 180 ug.l-1. Taste 24 to 135 ug.l-1. Threshold for tap water 20 to 40 ug.l-1.	<a href="http://www.advisorybodies.doh.gov.uk/comeap/statementsreports/mtbesupp.htm">http://www.advisorybodies.doh.gov.uk/comeap/statementsreports/mtbesupp.htm</a>	<a href="http://www.advisorybodies.doh.gov.uk/comeap/index.htm">www.advisorybodies.doh.gov.uk/comeap/index.htm</a>
European Chemicals Bureau (ECB)	2002	Drinking water	15	ug l-1	Odour and taste threshold in tap water. Maximum exposure anticipated within Private wells near petrol stations. No MTBE expected within municipal sources of drinking water. Combined Oral and Inhalation daily exposure is anticipated to be 21 ug.kg bw-1.d	<a href="http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf">http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf</a>	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>
IPCS Environmental Health Criteria (EHC) Monographs	1998	Drinking water	20	ug l-1	Concentration within drinking water below <20 ug.l-1 based on information from five US states	Zogorski JS, Morduchowitz A, Baehr AL, Bauman BJ, Drew RT, Korte NE, Lephram WW, Pankow JF, & Washington ER (1996) Fuel oxygenates and water quality: Current understanding of sources, occurrence in natural waters, environmental behaviour, fate, and sign	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>
WHO Guidelines for Drinking Water Quality	2006				A health-based guideline value has not been derived for MTBE, due to the fact that any guideline value that would be derived would be significantly higher than the concentration at which it would be detected by odour (15mg/litre is the lowest level elicit)	<a href="http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf</a>	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">www.who.int/water_sanitation_health/dwq/guidelines/en</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	25/03/2009	Drinking water	2.9	ug l-1	Average concentration in drinking water in the Netherlands generally very low <0.14 ug L-1, maximum 2.9 ug L-1.	<a href="http://www.rivm.nl/bibliotheek/rapporten/703719001.html">http://www.rivm.nl/bibliotheek/rapporten/703719001.html</a>	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>

<b>MTBE</b>		CAS 1634-04-4		Assessor A: Cheryl Davies, Delta-Simons	Assessor B: Sian Jones, Entec UK Ltd	Final Review:	Panel/SF
		Date	01/03/2009	Date	27/04/2009	Date	26/08/2009
Health Canada Toxicological Reference Values	2006	Drinking water	0.015	ug l-1	Based on odour detection levels. The limited available exposure data indicate that MTBE is unlikely to be found in Canadian drinking water supplies at levels that may pose risks to human health.	<a href="http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/water-eau/mtbe/mtbe-eng.pdf">http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/pubs/water-eau/mtbe/mtbe-eng.pdf</a>	<a href="http://www.hc-sc.gc.ca/index_e.html">www.hc-sc.gc.ca/index_e.html</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	1996	Groundwater wells	<20	ppb	Only 3% of wells in US urban areas exceeded 20 ppb	USGS. 1995. Occurrence of the gasoline additive MTBE in shallow ground water in urban and agricultural areas. Fact Sheet FS-114-95. United States Geological Survey, National Water-Quality Assessment (NAWQA) Program. (Available on World Wide Web).	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>
USEPA Health Advisories	Dec-97	Drinking water	20-40	ug l-1	Level of consumer acceptance	<a href="http://www.epa.gov/waterscience/criteria/drinking/mtbe.pdf">http://www.epa.gov/waterscience/criteria/drinking/mtbe.pdf</a>	<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
Other (UK Energy Institute)	2009	Drinking water	<0.5	ug l-1	94% of well fields sampled has less than detection limit (typically 0.5µg/L). Average intake calculated assuming 0.5µg/L, converted assuming 2L/day.	Energy Institute, 2009. Reported and Potential Occurrence of Ether Oxygenates on Water Resources in the UK.	N/A
<b>MDI</b>			<b>Recommended MDIinh</b>	<b>Units</b>	<b>Justification:</b> Based on COMEAP data. Ambient concentrations in UK air likely to be less than 10µg/m3. Converted to 200µg/day assuming an adult breathes 20m3/day.		
			200	ug day-1			

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Health and Safety Executive	2007	Workplace Air	92	mg.m-3	Long term (8hr) TWA. Occupational Exposure Limit	<a href="http://www.hse.gov.uk/coshh/table1.pdf">http://www.hse.gov.uk/coshh/table1.pdf</a>	<a href="http://www.hse.gov.uk">www.hse.gov.uk</a>
Committee on the Medical Effects of Air Pollutants (COMEAP)	2000	Air	30	ug.m-3	Levels in air likely to be <10 ug.m-3 (equivalent to 200µg/m3 assuming an adult breathes 20m3/day) Peak levels in air at petrol stations during refuelling 30 ug.m-3	<a href="http://www.advisorybodies.doh.gov.uk/comeap/statementsreports/mtbesupp.htm">http://www.advisorybodies.doh.gov.uk/comeap/statementsreports/mtbesupp.htm</a>	<a href="http://www.advisorybodies.doh.gov.uk/comeap/index.htm">www.advisorybodies.doh.gov.uk/comeap/index.htm</a>
European Chemicals Bureau (ECB)	24/06/1905	Air	29	mg.m-3	Maximum concentration exposed to for a couple of minutes at a time, 1-3 times a week, during refuelling	<a href="http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf">http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/mtbereport313.pdf</a>	<a href="http://ecb.jrc.it/">http://ecb.jrc.it/</a>
International Agency for Research on Cancer (IARC)	1999	Ambient air	4 to 20	ug.m-3	Ambient air concentrations in regions of US where MTBE-rich fuel is used	<a href="http://inchem.org/documents/iarc/vol73/73-13.html">http://inchem.org/documents/iarc/vol73/73-13.html</a>	<a href="http://inchem.org/pages/iarc.html">http://inchem.org/pages/iarc.html</a>
IPCS Environmental Health Criteria (EHC) Monographs	1998	Ambient air	14.4	ug.m-3	Concentrations within ambient air generally between 0.47 and 14.4 ug.m-3 (occasionally exceeding 35.7 mg.m-3 when refuelling). Literature review based on data from US, Canada and Finland	<a href="http://inchem.org/documents/ehc/ehc/ehc206.htm#PartNumber:3">http://inchem.org/documents/ehc/ehc/ehc206.htm#PartNumber:3</a>	<a href="http://inchem.org/pages/ehc.html">http://inchem.org/pages/ehc.html</a>
WHO Guidelines for Drinking Water Quality	2006				There have been a number of human studies of neurological and clinical effects of exposure to MTBE by inhalation, with mixed results. In general, no objective changes could be seen at levels of MTBE normally found, even in such microenvironments as gasoline	<a href="http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwq/gdwq0506.pdf</a>	<a href="http://www.who.int/water_sanitation_health/dwq/guidelines/en">www.who.int/water_sanitation_health/dwq/guidelines/en</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	2004	Oral and Inhalation?	0.004 to 0.005	mg.kg bw-1.d-1	Total background exposure from ECB (2002)	ECB (2002). European Union Risk Assessment Report t-butyl methyl ether. European Chemicals Bureau, 3rd Priority list, volume 19; Office for Official Publications of the EC, Luxembourg. Within <a href="http://www.rivm.nl/bibliotheek/rapporten/711701039.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701039.pdf</a>	<a href="http://www.rivm.nl/en/">www.rivm.nl/en/</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	1996	Ambient air	<0.2	ppb	Annual mean MTBE in ambient air in US in late 1980's	EPA. 1994c. Chemical summary for methyl-tert-butyl-ether. U. S. Environmental Protection Agency, Office of Pollution Prevention and Toxics. Washington, DC. EPA 749-F-94-017a. In <a href="http://www.atsdr.cdc.gov/toxprofiles/tp91.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp91.pdf</a>	<a href="http://www.atsdr.cdc.gov/">www.atsdr.cdc.gov/</a>

Substance: <b>Methyl tert-b utyl ether</b>		CAS Number: <b>1634-04-4</b>	Assessor A: <b>Siân Jones, Entec UK Ltd</b>	Assessor B: <b>Cheryl Davies, Delta-Simons</b>	Final Review: <b>Panel/SF</b>																					
Chemical Formula: <b>C<sub>5</sub>H<sub>12</sub>O</b>		Phase at Ambient Temperature: <b>Liquid</b>	Date: <b>31-Mar-09</b>	Date: <b>30-Apr-09</b>	Date: <b>26/08/2009</b>																					
Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	A		B		C		D		E		F		G		H						
						Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	Source Units	SR7 Units	
Required Parameters																										
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	88.1482	n/a	Median value chosen as central value of consistent range	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)			
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	7.18E+01	25	Median value chosen as central value of consistent range	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	4.80E+04	20	Median value chosen as central value of consistent range	mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
Chemical Boiling Point (ambient pressure)	K	n/a	3.28E+02	n/a	Median value chosen as central value of consistent range	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Chemical Melting Point (ambient pressure)	K	n/a	1.65E+02	n/a	Median value chosen as central value of consistent range	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
Log Octanol - Water Coefficient	Dimensionless	n/a	0.94	n/a	No consistent range - median value from most recent review chosen (Lide 2008)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	128	n/a	Single literature value	n/a	n/a	n/a	n/a	n/a	n/a	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	27733.51912	2.77E+04	Normal Chemical Boiling Point	Calculated value - similar to median value of consistent range	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Chemical Critical Point temperature (ambient pressure)	K	498.9366053	4.99E+02	n/a	Calculated value - similar to average from NIST source	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Critical Pressure	atm	33.67095454	3.37E+01	n/a	Calculated value - similar to average from NIST source	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	1.599E-02	10	Estimated from parameters above using Claypyron relationship or direct calculation
Vapour pressure at ambient soil temperature	Pa	18424.9561	10	Estimated from parameters above using Grain-Watson method
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	7.82E-06	10	Estimated from parameters above using Wilkie-Lee method
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	5.62E-10	10	Estimated from parameters above using Hayduk and Laudie method
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	1.53	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

<b>n-Butylbenzene</b>	<b>CAS Number:</b>	<b>104-51-8</b>	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panel/SF
			Date	15/04/2009	Date	06/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	No	Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.

<b>TDI oral</b>	<b>Recommended TDloral</b>	<b>Units</b>	<b>Justification</b>
	-	ug.kg-1.d-1	Insufficient data with sufficient detail on derivation to derive TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
USEPA PRG Region 9 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf</a>	2004	14/04/2009	Oral reference dose	4.00E-02	mg kg bw day <sup>-1</sup>	40	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/mediation/rrr.htm">http://www.tceq.state.tx.us/mediation/rrr.htm</a>	Mar-06	05/06/2009	Oral reference dose	4.00E-02	mg.kg day <sup>-1</sup>	40	Unknown	Unknown	Unknown

<b>TDI inhal</b>	<b>Recommended TDlinhal</b>	<b>Units</b>	<b>Justification</b>
	-	ug.kg-1.d-1	Insufficient data with sufficient detail on derivation to derive TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
USEPA PRG Region 9 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf</a>	2004	14/04/2009	Inhalation reference dose	4.00E-02	mg kg bw day <sup>-1</sup>	40	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/mediation/rrr.htm">http://www.tceq.state.tx.us/mediation/rrr.htm</a>	Mar-06	05/06/2009	Inhalation reference dose	7.80E-02	mg.kg day <sup>-1</sup>	78	Unknown	Unknown	Unknown

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**n-Butylbenzene**


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**TDI oral**

Organisation	Units	UF	UF description	Study type	Description	Target organ/Critical Effect	Reference	Web link
USEPA PRG Region 9 2004	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

**TDI inhal**

Organisation	Units	UF	UF description	Study type	Description	Response	Reference	Web link
USEPA PRG Region 9 2004	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

<b>n-Butylbenzene</b>	CAS 104-51-8	Assessor A: J Thornton, Golder Associates	Assessor B: N Dixon, WorleyParsons	Final review: Panel/SF
		Date: 16/04/2009	Date: 06/05/2009	Date: 28/08/2009

<b>MDIoral</b>	<b>Recommended MDIoral</b>	<b>Units</b>	<b>Justification:</b> No data, assumed negligible.
	0	ug day-1	
<b>MDlinh</b>	<b>Recommended MDlinh</b>	<b>Units</b>	<b>Justification:</b> Only data found
	5.4	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Toxicological Data Network (TOXNET)	06/05/2009	Indoor air	5.4	ug day-1	Mean indoor air measurements taken from non smoking homes (where study was carried out is not given)	Heavner DL et al; Environ Int 21: 3-21 (1995)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>



<b>Propylbenzene</b>	<b>CAS Number:</b>	<b>103-65-1</b>	<b>Assessor A:</b>	David Gallagher (ERM)	<b>Assessor B:</b>	Simon Clennell-Jones (WSP)	<b>Final review:</b>	Panel/SF
			<b>Date</b>	20/05/2009	<b>Date</b>	01/06/2009	<b>Date</b>	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	Carcinogenicity unclassified by IARC or USEPA. Toxicological data suggests it is unlikely to be a carcinogen. Insufficient data with sufficient detail on derivation to derive TDI.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral				Recommended TDloral	Units	Justification
				100	ug.kg-1.d-1	Ethylbenzene tox from EA 2009 TOX report. USEPA PPRTV recommend ethylbenzene tox for developing a "screening value" for Propylbenzene.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Feb-09	NA	RFD PPRTV	No chronic or sub chronic RFDs have been developed due to a lack of data. However, ethylbenzene toxicological data is recommended as a surrogate for propylbenzene for developing a "screening value". Ethylbenzene is considered to have similar patterns of absorptions, metabolism and neurological effects and considered to be more toxic than n-propylbenzene.										
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trppcls.html</a>	26/03/2009	19/05/2009	Threshold	4.00E-02	mg/kg/bw/day	40		unknown					unknown	RFD sourced from National Centre for Environmental Assessment (NCEA)

TDI inhal				Recommended TDlinhal	Units	Justification
				220	ug.kg-1.d-1	Ethylbenzene tox from EA 2009 TOX report. USEPA PPRTV recommend ethylbenzene tox for developing a "screening value" for Propylbenzene.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type	Description
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Feb-09	NA	RFC PPRTV	No chronic or sub chronic RFDs have been developed due to a lack of data. However, ethylbenzene toxicological data is recommended as a surrogate for propylbenzene fro developing a "screening value". Ethylbenzene is considered to have similar patterns of absorptions, metabolism and neurological effects and considered to be more toxic than n-propylbenzene.										
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	<a href="http://www.tceq.state.tx.us/remediation/trrp/trppcls.html">http://www.tceq.state.tx.us/remediation/trrp/trppcls.html</a>	26/03/2009	19/05/2009	Threshold	4.00E-01	mg/m <sup>3</sup>	114		unknown					unknown	RFC sourced from unidentified source

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**Propylbenzene**


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**TDI oral**


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Organisation	Target organ/Critical Effect	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)		Provisional Peer Reviewed Toxicity Values for n-Propylbenzene (CASRN 103-65-1).	NA
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 19th May 2009.	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppls.html</a>

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**TDI inhal**


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Organisation	Response	Reference	Web link
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)		Provisional Peer Reviewed Toxicity Values for n-Propylbenzene (CASRN 103-65-1).	NA
Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels	unknown	Texas Commission on Environmental Quality. Texas Risk Reduction Program Protective Concentration Levels. Accessed 19th May 2009.	<a href="http://www.tceq.state.tx.us/remediation/trrp/trrppls.html">http://www.tceq.state.tx.us/remediation/trrp/trrppls.html</a>

<b>Propylbenzene</b>	CAS 103-65-1	Assessor A:	David Gallagher (ERM)	Assessor B:	Simon Clennell-Jones (WSP)	Final review:	Panel/SF
		Date	20/05/2009	Date	01/06/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDIoral</b>	<b>Units</b>	<b>Justification:</b> No data, assumed negligible
	0	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
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<b>MDI</b>	<b>Recommended MDIinh</b>	<b>Units</b>	<b>Justification:</b> Based on the conservative end of the range reported by HSDB.
	16.44	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Toxicological Data Network (TOXNET)	11/08/2009	Urban / suburban air	12.1 - 16.44	ug/day	Assuming an avg n-propylbenzene concn of 0.605-0.822 ug/cu m in urban-suburban outdoor air and an inhalation rate of 20 cu m/day, the average daily intake is 12.1-16.44 ug/day (from USEPA National Ambient VOC database).	Hazardous Substances Databank (HSDB). Accessed through TOXNET on 11th August 2009	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>



sec-Butylbenzene	CAS Number:	135-98-8	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panel/SF
			Date	15/04/2009	Date	07/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	No	Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		
Apply IDinh to exposure routes?	No	No	No		Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.

TDI oral	Recommended TDloral	Units	Justification
			Insufficient data with sufficient detail on derivation to derive TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf</a>	2004	14/04/2009	Oral reference dose	4.00E-02	mg/kg-day	40	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/mediation/rrr.htm">http://www.tceq.state.tx.us/mediation/rrr.htm</a>	Mar-06	05/06/2009	Oral reference dose	4.00E-02	mg.kg day <sup>-1</sup>	40	Unknown	Unknown	Unknown

TDI inhal	Recommended TDlinhal	Units	Justification
			Insufficient data with sufficient detail on derivation to derive TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl e.pdf</a>	2004	14/04/2009	Inhalation reference dose	4.00E-02	mg/kg-day	40	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/mediation/rrr.htm">http://www.tceq.state.tx.us/mediation/rrr.htm</a>	Mar-06	05/06/2009	Inhalation reference dose	7.80E-02	mg.kg day <sup>-1</sup>	78	Unknown	Unknown	Unknown

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 sec-Butylbenzene
 

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 TDI oral
 

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Organisation	Units	UF	UF description	Study type	Description	Target organ/Critical Effect	Reference	Web link
USEPA Region 9 PRG 2004	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

 TDI inhal
 

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Organisation	Units	UF	UF description	Study type	Description	Response	Reference	Web link
USEPA Region 9 PRG 2004	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

<b>sec-Butylbenzene</b>	CAS 135-98-8	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panel/SF
		Date	15/04/2009	Date	06/05/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, assumed negligible.
	0	ug day-1	

<b>MDI</b>	<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Only value found (TOXNET), upper estimate used. Converted from data assuming 1ppb = 5.49µg/m <sup>3</sup> , and an adult breathes 20m <sup>3</sup> /day.
	5.4	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Toxicological Data Network (TOXNET)	14/04/2009	Ambient air	5.4	ug day-1	National survey of ambient air, which included five site types (remote, rural, suburban, urban, and source dominated) the average daily atmospheric concns of sec-butylbenzene was 0.033 and 0.049 ppb volume for 137 suburban and 279 urban samples, respectively. 1ppb = 5.49µg/m <sup>3</sup> , so 0.049ppb = 0.267µg/m <sup>3</sup> . Converted to 5.4µg/day assuming an adult breathes 20m <sup>3</sup> /day.	Shah JJ, Heyerdahl EK; National Ambient VOC Database Update USEPA-600/3-88/010 (1988)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

Substance:	sec butylbenzene	CAS Number:	135-98-8	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, Worley Parsons	Final Review:	Panel/SF
Chemical Formula:	C6H5CH(CH3)C2H5	Phase at Ambient Temperature	Liquid	Date:	16/04/2009	Date:	16/04/2009	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://ics3-hq.oecd.org/crpts/hpw/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990			B LIDE, 2008			C MACKAY et al. 2006			D MERCK, 2006			E MONTGOMERY, 2007			F MONTGOMERY, 1997			G NIST, 2005			H OECD, 2000					
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																																	
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	134.218	n/a	Median value in consistent range.		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)			
							no data	no data	n/a	134.218	134.218	n/a	134.218	134.218	n/a	134.218	134.218	n/a	134.22	134.22	n/a	no data	no data	n/a	134.22	134.22	n/a	no data	no data	n/a			
							atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	KPa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	Pa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)			
							no data	no data	25	1.89E+00	1.89E+03	25	1.40E+03	1400	25	n/a	n/a	n/a	1.14E-02	1.15E+03	25	no data	no data	25	1.39E+03	1.39E+03	25	no data	no data	25			
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	1.89E+03	25	No consistent range. Value from most recent source adopted.																												
							no data	no data	25	1.40E-02	14	25	3.09E+01	3.09E+01	25	no data	no data	25	1.76E+01	1.76E+01	25	no data	no data	25	2.00E+01	2.00E+01	10	no data	no data	10			
Solubility (S) 10 °C where possible. (Use unit converter if source provides different units)	mg/L	n/a	1.40E+01	25	Only source at 10 degrees (NIST) reported 20 mg/L but inconsistent with 25 degrees C data. No consistent range so most recent value from 25 degrees C data adopted.																												
							no data	no data	25	17.6	17.6	25	17.6	17.6	25	no data	no data	25	309	309	25	no data	no data	25	200	200	10	no data	no data	10			
Chemical Boiling Point (ambient pressure)	K	n/a	4.46E+02	n/a	Central value from a consistent range.		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							no data	#VALUE!	n/a	173.3	446.45	n/a	174	447.15	n/a	173.5	446.65	n/a	173.34	446.49	n/a	no data	#VALUE!	n/a	446	446.00	n/a	no data	#VALUE!	n/a	no data	#VALUE!	n/a
Chemical Melting Point (ambient pressure)	K	n/a	1.92E+02	n/a	Median value in consistent range.		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
							no data	no data	n/a	-82.7	190.45	n/a	-75	198.15	n/a	-82.7	190.45	n/a	-75.5	197.65	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
Log Octanol - Water Coefficient	Dimensionless	n/a	4.57	n/a	single source		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
							no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	4.57	4.57	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
Molar Volume (Le Bas method)	cm3 mol <sup>-1</sup>	n/a	1.85E+02	n/a	single source		n/a	n/a	n/a	n/a	n/a	n/a	cm3 mol <sup>-1</sup>	cm3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							no data	no data	n/a	184.8	184.80	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
Enthalpy of Vaporisation at normal boiling point (EVBVP)	J Mol <sup>-1</sup>	39740.31742	3.97E+04	n/a	Normal Chemical Boiling Point	Calculated Value	n/a	n/a	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
							no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
							no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
Chemical Critical Point temperature (ambient pressure)	K	650.9018071	650.9	n/a	Calculated Value	Calculated Value	n/a	n/a	n/a	K	K	Ref. Temp (C)	n/a	n/a	n/a	°C	K	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	
							no data	no data	n/a	652.5	652.50	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	
Critical Pressure	atm	28.90122254	28.90	not given	Calculated value	Calculated value	n/a	n/a	n/a	Bar	Atmosph	Ref. Temp (C)	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a		
							no data	no data	n/a	30.25	29.85442882	not given	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Recommended Literature Value	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	2.757E-01	n/a	Estimated from parameters above using Claypyon relationship or direct calculation
Vapour pressure at ambient soil temperature	Pa	88.40549908	n/a	Estimated from parameters above using Grain-Watson method
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	6.03E-06	n/a	Estimated from parameters above using Wilkie-Lee method
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	4.52E-10	n/a	Estimated from parameters above using Hayduk and Laudie method
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	3.80	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Styrene	CAS Number: 100-42-5	Assessor A: Nick Brown, Grontmij	Assessor B: Catherine Helm WD	Final Review: Panel/SF
	Date: 26/05/2009	Date: 01/06/2009	Date: 28/08/2009	

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	IARC has classified styrene as a Group 2B Carcinogen (possible human carcinogen). Potential carcinogenicity linked to styrene oxide. ATSDR concluded that humans have a high capacity to metabolise styrene oxide to styrene glycol and therefore low potential for carcinogenic activity from styrene. WHO concluded that potential genotoxic effects are not critical endpoints for development of HCVs. Health Council of the Netherlands concluded evidence for carcinogenicity in humans is weak and inconsistent. TDloral applied to oral and dermal routes. TDlinhal applied to inhalation route.
Apply IDoral to exposure routes?	No	No	No		
Apply TDinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	12	ug.kg-1.d-1	Value based on NOAEL of 12mg/kg bw/day identified by RIVM (Charles River rat study). An uncertainty factor of 1000 has been selected as recommended by SCF, IPCS, WHO, ATSDR and IRIS. Note that the WHO NOAEL has been incorrectly associated with the male rats and therefore the RIVM NOAEL (based on the same study) preferred.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Units	CLEA Units	ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>		05/05/2009	Stated that no HCV values are available	0.02mg/l Drinking water quality standard	mg/l									
		25/03/2009	31/03/2009	Acute oral toxicity rats, LD50 Acute oral toxicity mice, LD50	5000 rats 316 mice	mg/kg bw/day									
Health and Safety Executive (HSE)	<a href="http://www.hse.gov.uk/">http://www.hse.gov.uk/</a>		01/04/2009	Acute NOAEL		100 ppm									
HSE 2				Repeated dose NOAEL		200 ppm									Over 13 weeks in rats
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/ts/scf/index_en.htm">http://ec.europa.eu/food/ts/scf/index_en.htm</a>		05/05/2009	TDI for food		7.7 ug/kg-bw/day		7.7		NOAEL	7.7 mg/kg bw/day		1000	See WHO guidelines for DW	See WHO guidelines for DW
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	Published 2003	05/05/2009	TDI		7.7 ug/kg-bw/day		7.7		NOAEL	7.7 mg/kg bw/day		1000	x 100 for intra species and inter species variation and x 10 for carcinogenicity and genotoxicity of the intermeditation styrene-7,8-oxide	Charles River COBS CD 2 year study of drinking water in rats
IPCS INCHEM	<a href="http://incchem.org/">http://incchem.org/</a>		05/05/2009	TDI		0.04 mg/kg-bw/day		40		NOAEL	7.7 mg/kg bw/day		192.5 (Calculated from NOAEL level and value recommended)	Unclear - Basis for NOAEL specified as 7.7mg/kg/day in rats	Charles River COBS CD 2 year study of drinking water in rats
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	Published 2006	05/05/2009	TDI		7.7 ug/kg-bw/day		7.7		NOAEL	7.7 mg/kg bw/day		1000	x 100 for intra species and inter species variation and x 10 for carcinogenicity and genotoxicity of the intermeditation styrene-7,8-oxide	Charles River COBS CD 2 year study of drinking water in rats
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001	05/05/2009	TDI		120 ug/kg-bw/day		120		NOAEL	12 mg/kg bw/day		100	x 10 for interspecies variation, x 10 for intraspecies variation	2 year study of drinking water in rats
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>		05/05/2009	TDI		120 ug/kg-bw/day		120		NOAEL	12 mg/kg bw/day		100	x 10 for interspecies variation, x 10 for intraspecies variation	Beliles 1985: Sprague-Dawley Rat Study
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>		05/05/2009	Acute MRL		100 ug/kg/day		100		Acute Oral MRL			1000		
USEPA Acute Guideline Levels (AEGs)	<a href="http://epa.gov/oppt/aegl/pubs/chemlist.htm">http://epa.gov/oppt/aegl/pubs/chemlist.htm</a>	12/12/2006	09/04/2009	AEGs over 8 hours	20, 130, 340	ppm									
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Summer 2006	09/04/2009	RfD		0.2 mg/kg/day		200							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		05/05/2009	RfD		200 ug/kg-bw/day		200		NOAEL	200 mg/kg bw/day		1000	x 10 for interspecies variation, x 10 for intraspecies variation, x 10 sub-chronic to chronic	Quast Dog Study
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>		05/05/2009	RfD	as above	as above	as above	as above	as above	as above	as above	as above	as above	as above	as above

## Styrene

TDI oral				
Organisation	Description	Target organ/Critical Effect	Reference	Web link
Health Protection Agency (HPA)	Toxic by inhalation, ingestion and skin contact. Possible human carcinogen and cause of CNS depression.	Irritation to any tissues contacted. Limited evidence from animal studies that styrene will cause adverse effects on reproduction.	HPA Compendium of Chemical Hazards, Styrene. JC Wakefield, HPA 2008	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1202115635291">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1202115635291</a>
		Rats - increased liver and kidney weights, growth depression		
Health and Safety Executive (HSE)		CNS depression, skin, eye and respiratory tract irritation, repeated dose toxicity	?????	????
HSE 2		CNS depression, skin, eye and respiratory tract irritation, repeated dose toxicity	????	????
Scientific Committee on Food (SCF) pre 2002	See WHO guidelines for DW	See WHO guidelines for DW	WHO (1993). Guidelines for drinking water guidelines, 2 <sup>nd</sup> edition, vol. 1. Health criteria and other supporting information. World Health Organization, Geneva.	<a href="http://ec.europa.eu/food/fs/sc/scf/out24_en.html">http://ec.europa.eu/food/fs/sc/scf/out24_en.html</a>
International Programme on Chemical Safety (IPCS)	2 year oral study rats received 0, 125mg/l and 250mg/l in drinking water. At 250mg/l females showed lower terminal body weight than lower dose groups. 125mg/l identified as an NOAEL equating to 7.7mg/kg (males) and 12mg/kg (females)	Reduced body weight	Styrene in Drinking Water. Background Document for the development of WHO Guidelines for Drinking-water Quality. World Health Organisation 2003 Primary (Study) Reference given as: Chemical Manufacturers Association (1980) Toxicological study on styrene incorporated in drinking water of rats for two years in conjunction with three generation reproduction study. Litton Bionetic	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/styrene.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/styrene.pdf</a>
IPCS INCHEM	As above	As Above	Primary Reference given as: Chemical Manufacturers Association (1980) Toxicological study on styrene incorporated in drinking water of rats for two years in conjunction with three generation reproduction study. Litton Bionetics	<a href="http://www.inchem.org/documents/ecfa/ecfmono/v19ie15.htm">http://www.inchem.org/documents/ecfa/ecfmono/v19ie15.htm</a>
WHO Guidelines for drinking water Quality	2 year oral study rats received 0, 125mg/l and 250mg/l in drinking water. At 250mg/l females showed lower terminal body weight than lower dose groups. 125mg/l identified as an NOAEL equating to 7.7mg/kg (males) and 12mg/kg (females)	Reduced body weight	Guidelines for Drinking-water Quality. First Addendum to the Third Edition. Volume 1, Recommendations. World Health Organisation 2006 Principal Reference: Styrene in Drinking Water. Background Document for the development of WHO Guidelines for Drinking-water Quality. World Health Organisation 2003	<a href="http://www.who.int/water_sanitation_health/dwg/gdwq0506.pdf">http://www.who.int/water_sanitation_health/dwg/gdwq0506.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	2 year oral study rats received 0, 125mg/l and 250mg/l in drinking water. At 250mg/l females showed lower terminal body weight than lower dose groups. 125mg/l identified as an NOAEL for females. Males showed no effects at 250mg/l (NOAEL). i.e.. This is the same study but different interpretation of the results from the WHO approach above	Reduced body weight in females	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001 (Primary Reference given as Van Apeldorn et al. 1986)	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
Health Canada Toxicological Values	Dose groups of 125mg/l and 250 mg/l in drinking water. Over three generations. 125mg/l identified as NOAEL. 250mg/l as LOAEL	Reproductive effects in three generation rat study	Primary (Study) Reference: Beliles et al. 1985	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/stryene/styrene_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/stryene/styrene_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels				<a href="http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf">http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf</a>
USEPA Acute Guideline Levels (AEGs)				?????
USEPA Health Advisors				
USEPA Integrated Risk Information System (IRIS)	Four beagle dogs/sex were gavaged with doses of 0, 200, 400, or 600 mg styrene/kg bw/day in peanut oil for 560 days. No adverse effects were observed for dogs administered styrene at 200 mg/kg-day.	Red blood cell and liver effects	Quast, J.F., C.G. Humiston, R.Y. Kalnins, et al. 1979. Results of a toxicity study of monomeric styrene administered to beagle dogs by oral intubation for 19 months. Toxicology Research Laboratory, Health and Environmental Sciences, DOW Chemical Co., Midland, MI. Final Report.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/?./temp/~wxAHsQ:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/?./temp/~wxAHsQ:1</a>
Toxicology Data Network (Toxnet)	as above	as above	as above	as above

Styrene	CAS Number: 100-42-5	Assessor A: Nick Brown, Grontmij	Assessor B: Catherine Helm WD	Final Review: Panel/SF
	Date: 26/05/2009	Date: 01/06/2009	Date: 28/08/2009	

TDI inhal	Recommended TDIinhal: 240	Units: ug.kg-1.d-1	Justification: ATSDR value has been selected because of relevance and quality of study but primary reference is still draft. However the second best source (RIVM) used the original ATSDR Toxicological Profile (1993) which is slightly less conservative. i.e. More conservative draft value has been selected
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Organisation	Last Updated	Health criteria type	Value	Units	CLEA Units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description	Study type
Health Protection Agency (HPA)	<a href="http://www.hpa.org.uk/">http://www.hpa.org.uk/</a>	05/05/2009	WHO Air Quality Guideline	0.26 (weekly average)	mg/m3	74						
Health Protection Agency (HPA)	25/03/2009	31/03/2009	4 hour LC50	2700	mg/m3							Rats
Health Protection Agency (HPA)	25/03/2009	31/03/2009	2 hour LC50	2160	mg/m3							Mice
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	05/05/2009	TCA	900	ug/m3	257	NOAEC	26 (107)	mg/m3		30 x 3 for LOAEC to NOAEC 10 for intra human variation	x Occupational exposure assessment
Health Canada Toxicological Values	<a href="http://www.hc-sc.gc.ca/index_e.html">http://www.hc-sc.gc.ca/index_e.html</a>	05/05/2009	TDI	41	ug/kg bw/day	41	LOAEL	260	mg/m3		500 x 5 for LOEL, x 10 for interspecies variation, x 10 for intraspecies	Kishi Study: Wistar Rats
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	05/05/2009	MRL	0.2	ppm (1ppm = 4.25mg/m3)	240	LOAEL from Metanalysis of data	20	ppm		100 10 LOAEL and 10 Intra Species Variation	Occupational Exposure studies
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>	05/05/2009	RFC	1	mg/m3	285	NOAEL	30	mg/m3		30 x 3 database inadequacies X10 intra-species variation	Mutti et al. (1984)
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	as IRIS	as IRIS	as IRIS	as IRIS	as IRIS	as IRIS			as IRIS	as IRIS	as IRIS

## Styrene

TDI inhal				
Organisation	Description	Response	Reference	Web link
Health Protection Agency (HPA)		Long term human exposure to Styrene reported to cause subtle changes in hearing, balance, colour vision, psychological performance and asthma	HPA Compendium of Chemical Hazards, Styrene. JC Wakefield, HPA 2008	<a href="http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1202115635291">http://www.hpa.org.uk/web/HPAwebFile/HPAweb_C/1202115635291</a>
Health Protection Agency (HPA)				
Health Protection Agency (HPA)				
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Minor effects on the central nervous system observed in humans exposed to 107mg/m3 of styrene for a period of several years. 107mg/m3 can be converted to 26mg/m3 to account for continuous exposure	Liver Weight, Serum Enzyme Levels and neurological effects	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001 (Primary Reference given as: Toxicological Profile for Styrene, ATSDR 1992)	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
Health Canada Toxicological Values	Offspring exposed to 60 to 293 ppm for 6 hrs/day during days 7 to 21 days of gestation	Reduced weight of offspring	Primary Reference: Kishi et al. 1992a, 1992b	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psi1-lsp1/stryene/styrene_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/psi1-lsp1/stryene/styrene_3-eng.php</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Analysis of data recorded from several studies including Kishi et al. (2001) and Mutti et al. (1984)	Choice Reaction Time and Colour Recognition	ATSDR, Toxicological Profile for Styrene. Draft for Public Comment. September 2007 Primary Study Reference: Benignus et al. 2005, Human neurobehavioral effects of long-term exposure to Styrene: a Meta-analysis. Environmental Health Perspect 113: 532-538	<a href="http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf">http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf</a>
USEPA Integrated Risk Information System (IRIS)	Styrene occupational exposure was assessed by the authors to correspond to air concentrations ranging from 10-300 ppm as a mean daily exposure.	neuropsychological	Mutti, A., A. Mazzucchi, P. Rusticelli, G. Frigeri, G. Arfini, and I. Franchini. 1984. Exposure-effect and exposure-response relationships between occupational exposure to styrene and neuropsychological functions. Am. J. Ind. Med. 5: 275-286.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/?/temp/~crTanp:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/?/temp/~crTanp:1</a>
Toxicology Data Network (Toxnet)	as IRIS	as IRIS	as IRIS	as IRIS

<b>Styrene</b>	CAS 100-42-5	Assessor A: Nick Brown Grontmij	Assessor B: Catherine Helm WD Environmental	Final Review	Panel/SF
		Date: 29/05/2009	Date: 01/06/2009	Date:	28-Aug-09

<b>MDI</b>	<b>Recommended MDIoral</b>	<b>Units</b>	<b>Justification:</b> Value selected is the average intake predicted by the Styrene Working Group (in 1983) (JECFA). Value is UK specific and considered likely to be conservative.
	1	ug day-1	

Organisation	Date	Media	Value	Units	Description	Reference	Web link
Health Protection Agency	31/03/2009				Exposure from residues in plastics & natural environment likely to be extremely low. Most exposure in workplace.		<a href="http://www.who.int/water_sanitation_health/dwa/chemicals/styrene.pdf">http://www.who.int/water_sanitation_health/dwa/chemicals/styrene.pdf</a>
European Chemicals Bureau (ECB)	31/03/2009	Drinking Water	nd to 0.25 & 0.1, 0.3, 0.5	ug/l	Treated DW Ontario 1988-1990, 86 sources & Great Lakes Canada, 1982-1983, Avs for summer, winter, spring	European Risk Assessment Report, Styrene, Part 1 Environment. Institute for Health and Consumer Protection and the European Chemicals Bureau, 2002	<a href="http://ecb.irc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/styrenereport034.pdf">http://ecb.irc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/styrenereport034.pdf</a>
		Plastic-wrapped food	<1 - 200ug/kg, mostly <10ug/kg & 26% <1ug/kg	ug/kg	UK Study (Glibert & Startin in 1983)		
		Food	beer 10-200; coffee 20-360; bilberries 25; blackcurrants 60	ug/kg	UK Study by Miller et al 1994		
		Plastic-wrapped food	10 to 26; <1 to 223	ug/kg	MAFF in 1983, dairy products; MAFF in 1992 & 1994		
		Unwrapped food - cinnamon	157-39, 200	ug/kg	UK Study by Miller et al 1994		
		Unwrapped food	0.3-6.1	ug/kg	UK Study by Miller et al 1994		
		Water	10	ug/l	Reasonable value for water, based on review of potential sources		
Food	0.019	mg/kg bw/day	Sum of fish (Canadian), milk (UK) & other (UK), includes air				
Joint Expert Committee on Food Additives (JECFA)	31/03/2009	UK dietary intake	1 (average intake) 4 (Maximum Likely Intake)	ug/day	UK study of dietary intake. Styrene concentrations were measured in a range of foods that had come into contact with styrene polymers or co-polymers. Concentrations of styrene within individual food samples ranged between <1 and 205ug/kg. Average intakes and maximum likely intakes were calculated by multiplying average and maximum concentrations by the estimated mass of daily consumption for specific food types (as estimated during an earlier study by the Styrene Working Group)	Primary reference: Survey of styrene levels in food contact materials and in food. The eleventh report of the Steering Group on Food Surveillance. London, Ministry of Agriculture, Fisheries and Food, 1983 (Food Surveillance Paper, No. 11)	<a href="http://ec.europa.eu/food/fs/sc/scf/out24_en.html">http://ec.europa.eu/food/fs/sc/scf/out24_en.html</a>
International Programme on Chemical Safety (IPCS)	31/03/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	<a href="http://www.who.int/water_sanitation_health/dwa/chemicals/styrene.pdf">http://www.who.int/water_sanitation_health/dwa/chemicals/styrene.pdf</a>
	31/03/2009						
Joint Expert Committee on Food Additives (JECFA)	31/03/2009	See WHO Air Quality Guidelines for Europe	See WHO Air Quality Guidelines for Europe	See WHO Air Quality Guidelines for Europe	See WHO Air Quality Guidelines for Europe	See WHO Air Quality Guidelines for Europe	<a href="http://www.euro.who.int/document/aia/5_12styrene.pdf">http://www.euro.who.int/document/aia/5_12styrene.pdf</a>
	31/03/2009						

Styrene	CAS 100-42-5	Assessor A: Nick Brown Grontmij Date: 29/05/2009	Assessor B: Catherine Helm WD Environmental Date: 01/06/2009	Final Review Date: 28-Aug-09	Panel/SF		
WHO Guidelines for Drinking Water Quality	31/03/2009	Food and drinking water	5	ug/day	WHO data based on typical intake of 500g of milk products in styrene based packaging. Drinking water exposure is recorded as low (<1ug/l in drinking water in the US).	WHO (1996) Styrene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/27)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/styrene.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/styrene.pdf</a>
	31/03/2009	Total exposure	40	ug/day	Estimated value of total exposure for non-smokers in non-industrial areas		
WHO Air Quality Guidelines for Europe	31/03/2009	Food and drinking water	1 to 4	ug/day	UK Dietary Sources (Range of 1 - 4 is provided)	WHO 2000, Air Quality Guidelines - Second Edition Primary source is cited as: Survey of styrene levels in food contact materials and in food. The eleventh report of the Steering Group on Food Surveillance. London, Ministry of Agriculture, Fisheries and Food, 1983 (Food Surveillance Paper, No. 11)	<a href="http://www.euro.who.int/document/aiaq/5_12styrene.pdf">http://www.euro.who.int/document/aiaq/5_12styrene.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	31/03/2009	Food sources	0	ug/l	Intake from food sources assumed to be minimal in the Netherlands	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
Health Canada Toxicological Values	31/03/2009	Drinking Water	0.05 - 0.250	ug/l	80 drinking water supplies tested during Ontario's 1990 Drinking Water Surveillance	Primary Reference cited as Lachmaniuk, 1991	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/styrene/styrene_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/styrene/styrene_3-eng.php</a>
			0	ug/l	trace concentrations only in 1 of 1081 samples tested from 220 locations	Primary Reference cited as Halina, 1992	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	31/03/2009	Water	0	ug/day	Rarely detected in soil and drinking water samples in the USA. Estimates of intake via food not provided	ATSDR, Toxicological Profile for Styrene. Update. Draft for Public Comment. September 2007	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp53.html">http://www.atsdr.cdc.gov/toxprofiles/tp53.html</a>
USEPA Health Advisories	31/03/2009	DW	0.07	mg/l	MCLG & MCL		<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>
Toxicological Data Network (TOXNET)	31/03/2009		ND to 2,277	ug/l	ADI from water in HSDB Database (trans isomer)	USEPA; National Contaminant Occurrence Database. trans-1,2-Dichloroethylene. Available from the Database Query page at <a href="http://www.epa.gov/safewater/data/ncod.html">http://www.epa.gov/safewater/data/ncod.html</a> as of Apr 12, 2001.	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>

Organisation	Date	Media	Value	Units	Description	Reference	Web link
European Chemicals Bureau (ECB)	14/04/2009	Ambient air	0.59 (Mean of all values)	ug/m3	1988-1990 Canadian Study of Urban Air - Largest study identified and assumed to be representative by ECB. Maximum of 2.35ug/m3 identified	European Risk Assessment Report, Styrene, Part 1 Environment. Institute for Health and Consumer Protection and the European Chemicals Bureau, 2002	<a href="http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/styrenereport034.pdf">http://ecb.jrc.ec.europa.eu/Documents/Existing-Chemicals/RISK_ASSESSMENT/REPORT/styrenereport034.pdf</a>
		Urban US air	2.165	ug/m3	Industrial complex in Houston close to major transport routes 1987-88. Mean concentration identified by Lagrone, 1991		
		Urban Dutch air	mean <0.43, max 3	ug/m3	Urban Dutch air as identified by Bos et al., 1977		
		Urban Japanese air	0.43-1.7	ug/m3	Levels in Japanese air identified by Hoshika 1977		
Joint Expert Committee on Food Additives (JECFA)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	<a href="http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf</a>
WHO Guidelines for Drinking Water Quality	14/04/2009	Industrial Air	400	ug/day	Further detail not provided	WHO (1996) Styrene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/27)	<a href="http://www.who.int/water_sanitation_health/dwg/chemicals/styrene.pdf">http://www.who.int/water_sanitation_health/dwg/chemicals/styrene.pdf</a>
	14/04/2009	Air - through traffic pollution	10 to 50	ug/day			
	14/04/2009	open air	2	ug/day			
WHO Air Quality Guidelines for Europe	14/04/2009	Indoor Air	0.28	ug/m3	National Pilot Study in Canadian Homes (757 homes). NB. the mean concentration is misquoted as 280ug/m3 however the correct value can be found within the following reference: Exposure to Styrene in the General Canadian Population, Newhook R & Caldwell I, IARC Sci. Publication, 1993; 127, 27-33	WHO Regional Office for Europe, Copenhagen, Denmark. 2000, Air Quality Guidelines 2nd Edition Primary reference cited as Newhook, R. & Caldwell, K.. Exposure to styrene in the general Canadian population. In: Sorsa, M et al. Butadiene and Styrene: assessment of health hazards. Lyon, International Agency for Research on Cancer, 1993, pp. 27-33 (IARC Scientific Publications. No. 127)	<a href="http://www.euro.who.int/document/aiaq/5_12styrene.pdf">http://www.euro.who.int/document/aiaq/5_12styrene.pdf</a>
		Ambient air	0.09 - 2.35	ug/m3	Mean concentrations recorded at 18 sites in 5 provinces		

Styrene		CAS 100-42-5		Assessor A: Nick Brown Grontmij	Assessor B: Catherine Helm WD Environmental	Final Review	Panel/SF
		Date	Date	Date	Date	Date	Date
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Air	5	ug/kg-bw/day	Inhalation of air is assumed to account for all significant intake of Styrene in the Netherlands	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
Health Canada Toxicological Values	14/04/2009	Indoor Air	0.28	ug/m3	National Pilot Study in Canadian Homes (757 homes). NB. the mean concentration is misquoted as 280ug/m3 on the Health Canada Website however the correct value can be found within the following reference: Exposure to Styrene in the General Canadian Population, Newhook R & Caldwell I, IARC Sci. Publication, 1993; 127, 27-33	Primary Reference cited as Concord Environmental, 1992	<a href="http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/styrene/styrene_3-eng.php">http://www.hc-sc.gc.ca/ewh-semt/pubs/contaminants/ps1-lsp1/styrene/styrene_3-eng.php</a>
	14/04/2009	Ambient air	0.09 - 2.35	ug/m3	Mean concentrations recorded at 18 site in 5 provinces	Primary Reference cited as Dann, 1990	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Ambient air	0.11-0.36	ug/m3	Concentrations recorded in Chilba City Japan by Uchiyama and Hasegawa (2000)	ATSDR, Toxicological Profile for Styrene. Update. Draft for Public Comment. September 2007	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp53.html">http://www.atsdr.cdc.gov/toxprofiles/tp53.html</a>
	14/04/2009	Ambient air	0.1	ug/m3	Average concentration recorded in Minnesota (Pratt et al. 200) Median concentration was 0.08 and maximum was 1.49		
		Indoor air	0.1-50	ug/m3	Estimate: Primary data source unclear		
Toxicological Data Network (TOXNET)	31/03/2009	Polluted urban air	400	ug/day	Estimate of nominal ADI - US.	IARC Monographs on the Evaluation of Carcinogenic Risks to Humans. Geneva, Switzerland: World Health Org, Inter Agency Res Cancer. 60: 248 (1994)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>
		Urban air	6	ug/day			
		Indoor air	6-1000	ug/day			



tert-Butylbenzene	CAS Number:	98-06-6	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panel/SF
			Date	15/04/2009	Date	07/05/2009	Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	No	No	No	No	Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	No		Insufficient data with sufficient detail on derivation to derive TDI. No data regarding human carcinogenicity.
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
			Insufficient data with sufficient detail on derivation to derive TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabe.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabe.pdf</a>	2004	14/04/2009	Preliminary Remediation Goal	4.00E-02	mg/kg-day	40	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.htm">http://www.tceq.state.tx.us/remediation/rrr.htm</a>	Mar-06	05/06/2009	Oral reference dose	4.00E-02	mg.kg day <sup>-1</sup>	40	Unknown	Unknown	Unknown

TDI inhal	Recommended TDlinhal	Units	Justification
			Insufficient data with sufficient detail on derivation to derive TDI.

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value
USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabe.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabe.pdf</a>	2004	14/04/2009	Inhalation reference dose	4.00E-02	mg/kg-day	40	Unknown	Unknown	Unknown
Texas Commission on Environmental Quality	<a href="http://www.tceq.state.tx.us/remediation/rrr.htm">http://www.tceq.state.tx.us/remediation/rrr.htm</a>	Mar-06	05/06/2009	Oral reference dose	7.80E-02	mg.kg day <sup>-1</sup>	78	Unknown	Unknown	Unknown

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**tert-Butylbenzene**


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**TDI oral**


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Organisation	Units	UF	UF description	Study type	Description	Target organ/Critical Effect	Reference	Web link
USEPA Region 9 PRG 2004	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

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**TDI inhal**


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Organisation	Units	UF	UF description	Study type	Description	Response	Reference	Web link
USEPA Region 9 PRG 2004	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	USEPA Region 9 PRG 2004	<a href="http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf">http://www.epa.gov/region09/superfund/prg/files/04prgtabl_e.pdf</a>
Texas Commission on Environmental Quality	Unknown	Unknown	Unknown	Unknown	Unknown	Unknown	Texas Commission on Environmental Quality- Clean up standards	<a href="http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls">http://www.tceq.state.tx.us/assets/public/remediation/rrr/rrrtoxchph_2006.xls</a>

<b>tert-Butylbenzene</b>	CAS 98-06-6	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, WorleyParsons	Final review:	Panel/SF
		Date	16/04/2009	Date	06/05/2009	Date	28/08/2009

<b>MDI</b>	<b>Recommended MDI<sub>oral</sub></b>	<b>Units</b>	<b>Justification:</b> No data, assumed negligible.
	0	ug day <sup>-1</sup>	

<b>MDI</b>			<b>Recommended MDI<sub>inh</sub></b>	<b>Units</b>	<b>Justification:</b> Only data found, UK specific (TOXNET). Converted assuming an adult breathes 20m <sup>3</sup> /day.		
			780	ug day <sup>-1</sup>			
<b>Organisation</b>	<b>Date</b>	<b>Media</b>	<b>Value</b>	<b>Units</b>	<b>Description</b>	<b>Reference</b>	<b>Web link</b>
Toxicological Data Network (TOXNET)	14/04/2009	Ambient air	780	ug day <sup>-1</sup>	0- 39 ug.m <sup>3</sup> study carried out in 1979 in 6 cities surrounding Gatwick airport London. Converted using 39µg/m <sup>3</sup> x 20m <sup>3</sup> /day.	Tsani-Bazaca E et al; Chemosphere 11: 11-23 (1982)	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~H43sxi:1">http://toxnet.nlm.nih.gov/cgi-bin/sis/search/f?/.temp/~H43sxi:1</a>

Substance:	<b>tert butylbenzene</b>	CAS Number:	98-06-6	Assessor A:	J Thornton, Golder Associates	Assessor B:	N Dixon, Worley Parsons	Final Review:	Panel/SF
Chemical Formula:	<b>C10H14</b>	Phase at Ambient Temperature	Liquid	Date:	16/04/2009	Date:	06/05/2009	Date:	28/08/2009

<http://srdata.nist.gov/solubility/>  
<http://webbook.nist.gov/chemistry/>  
<http://cs3-hq.oecd.org/scripts/hpw/>

Property	Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale	References	A HOWARD, 1990		B LIDE, 2008		C MACKAY et al, 2006		D MERCK, 2006		E MONTGOMERY, 2007		F MONTGOMERY, 1997		G NIST, 2005		H OECD, 2000			
							Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)
<b>Required Parameters</b>																								
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	134.218	n/a	Most values are the same, most accurate		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)
						Average	no data	no data	n/a	134.218	134.218	n/a	134.218	134.218	n/a	134.22	134.22	n/a	134.22	134.22	n/a	134.22	134.22	n/a
							atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	KPa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	Pa m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)	atm m3 mol <sup>-1</sup>	Pa m3 mol <sup>-1</sup>	Ref. Temp (C)
Henry's Law Constant (HLC)	Pa m3 mol <sup>-1</sup>	n/a	1.28E+03	25	No consistent range, value from most recent source adopted		no data	no data	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25
						Geomean	no data	no data	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25	1.28E+03	1.28E+03	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	2.73E+01	25	Median value of consistent range		no data	no data	25	3.20E-02	3.70E+01	25	3.40E+01	3.40E+01	25	2.95E+01	2.95E+01	25	no data	no data	25	3.40E+01	3.40E+01	25
						Geomean	no data	no data	25	3.20E-02	3.70E+01	25	3.40E+01	3.40E+01	25	2.95E+01	2.95E+01	25	no data	no data	25	3.40E+01	3.40E+01	25
Chemical Boiling Point (ambient pressure)	K	n/a	4.42E+02	n/a	Median value from a consistent range.		no data	no data	n/a	169.1	442.25	n/a	169	442.15	n/a	168.5	441.65	n/a	169.15	442.30	n/a	no data	no data	n/a
						Average	no data	no data	n/a	169.1	442.25	n/a	169	442.15	n/a	168.5	441.65	n/a	169.15	442.30	n/a	no data	no data	n/a
Chemical Melting Point (ambient pressure)	K	n/a	2.15E+02	n/a	Median value from a consistent range.		no data	no data	n/a	-57.8	215.35	n/a	-75	198.15	n/a	-58	215.15	n/a	-57.8	215.35	n/a	no data	no data	n/a
						Average	no data	no data	n/a	-57.8	215.35	n/a	-75	198.15	n/a	-58	215.15	n/a	-57.8	215.35	n/a	no data	no data	n/a
Log Octanol - Water Coefficient	Dimensionless	n/a	4.11	n/a	Median value from consistent range		no data	no data	n/a	4.11	4.11	n/a	4.11	4.11	n/a	4.11	4.11	n/a	4.11	4.11	n/a	no data	no data	n/a
						Average	no data	no data	n/a	4.11	4.11	n/a	4.11	4.11	n/a	4.11	4.11	n/a	4.11	4.11	n/a	no data	no data	n/a
Molar Volume (Le Bas method)	cm3 mol <sup>-1</sup>	n/a	1.85E+02	n/a	single source		no data	no data	n/a	184.8	184.80	n/a	184.8	184.80	n/a	184.8	184.80	n/a	184.8	184.80	n/a	no data	no data	n/a
						Average	no data	no data	n/a	184.8	184.80	n/a	184.8	184.80	n/a	184.8	184.80	n/a	184.8	184.80	n/a	no data	no data	n/a
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	37728.14046	3.77E+04	n/a	Normal Boiling Point		no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	47.72	47720	n/a
						Average	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	47.72	47720	n/a
Chemical Critical Point temperature (ambient pressure)	K	652.9823193	653.0	n/a	Calculated Value		no data	no data	n/a	647.5	647.50	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a
						Average	no data	no data	n/a	647.5	647.50	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a
Critical Pressure	atm	28.90122254	28.90	not given	Calculated Value		no data	no data	n/a	29	28.62077473	not given	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a
						Average	no data	no data	n/a	29	28.62077473	not given	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a	no data	no data	n/a

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Recommended Literature Value	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> .cm <sup>-3</sup>	1.998E-01	n/a	Estimated from parameters above using Claypon relationship or direct calculation

Property	Units	Calculated Value	Recommended Literature Value	Rationale
Vapour pressure at ambient soil temperature	Pa	143.5025549	n/a	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Recommended Literature Value	Rationale
Diffusion coefficient in air	m <sup>2</sup> .s <sup>-1</sup>	6.04E-06	n/a	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Recommended Literature Value	Rationale
Diffusion coefficient in water	m <sup>2</sup> .s <sup>-1</sup>	4.52E-10	n/a	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Recommended Literature Value	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> .g <sup>-1</sup>	3.43	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Trans 1,2 Dichloroethene	CAS Number:	156-60-5	Assessor A:	Nick Brown, Grontmij	Assessor B:	Catherine Helm, WD Environmental	Final Review:	Panel/SF
	Date	26/05/2009	Date		Date		Date	28/08/2009

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	No	RIVM have evaluated the carcinogenicity of trans-1,2-dichloroethylene. RIVM concluded that trans-1,2-dichloroethylene was negative in in vivo genotoxicity tests but induced aneuploidy in in vitro tests. However, RIVM concluded that with induction of this type of genotoxic effect, a threshold approach (i.e., TDI) is appropriate. ATSDR did not identify any studies of potential carcinogenicity in animals or plants. TDloral applied to oral and dermal routes. TDlinh applied to inhalation route.
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral					Recommended TDloral	Units	Justification						
					17	ug.kg-1.d-1	Value conforms with WHO, RIVM and IRIS. All are based on the using Barnes Study and a UF of 1000. ATSDR use the same study but have adopted a lower UF						
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA Value (ug.kg-1.d-1)	Confidence rating	Basis	Value	Units	UF	UF description
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	Published 2003	28/04/2009	TDI	17	ug/kg/bw	17		NOAEL	17	mg/kg-bw/day	1000	x10 inter species, x 10 intra species, x 10 limited study duration
Joint Expert Committee on Food Additives (JECFA)	<a href="http://who.int/ipcs/food/iecf/en/">http://who.int/ipcs/food/iecf/en/</a>	Published 2003	28/04/2009	TDI	17	ug/kg/bw	17		NOAEL	17	mg/kg-bw/day	1000	x10 inter species, x 10 intra species, x 10 limited study duration
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001	28/04/2009	TDI	17	ug/kg/bw	17	medium reliability	NOAEL	17	mg/kg-bw/day	1000	x10 inter species, x 10 intra species, x 10 limited study duration
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>	Published 2008	28/04/2009	Oral Minimum Risk Level (int)	200	ug/kg/day	200		NOAEL	17	mg/kg-bw/day	100	x10 inter species, x 10 intra species
USEPA Acute Guideline Levels (AEGs)	<a href="http://epa.gov/oppt/aegl/pubs/chemlist.htm">http://epa.gov/oppt/aegl/pubs/chemlist.htm</a>	8.12.99	14.4.09	8-hour AEGs	280,450,620	ppm							
USEPA Health Advisors	<a href="http://www.epa.gov/waterscience/criteria/drinking">http://www.epa.gov/waterscience/criteria/drinking</a>	Summer 2006	14.4.09	MCLG & MCL	0.1	mg/l							
USEPA Integrated Risk Information System (IRIS)	<a href="http://epa.gov/iris/">http://epa.gov/iris/</a>		28/04/2009	Oral RfD	0.02	mg/kg/day	20	Study - medium database - low - low	NOAEL	17	mg/kg-bw/day	1000	x10 inter species, x 10 intra species, x 10 limited study duration
Toxicology Data Network (Toxnet)	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>		28/04/2009	See IRIS above	See IRIS above	See IRIS above	See IRIS above	See IRIS above	See IRIS above	17	mg/kg-bw/day	See IRIS above	See IRIS above

TDI inhalation					Recommended TDloral	Units	Justification						
					17	ug.kg-1.d-1	Value provided by RIVM and US EPA PPRTV using Freundt Study and a UF of 3000						
Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA Value (ug.kg-1.d-1)	Confidence rating	Basis	Value	Units	UF	UF description
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	Published 2001	28/04/2009	Provisional TCA (tolerable concentration in air)	60	ug/m3	17	low reliability	LOAEL	185	mg/m3	3000	x10 inter species, x 10 intra species, x 10 limited study duration x 3 for use of LOAEL
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	<a href="http://www.atsdr.cdc.gov/">http://www.atsdr.cdc.gov/</a>		02/04/2009	MRL Int/Acute	0.2	ppm	51.4		LOAEL	185	mg/m3	1000	x10 inter species, x 10 intra species, x 10 for use of LOAEL
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	<a href="http://rais.ornl.gov/tox/unauthorized.shtml">http://rais.ornl.gov/tox/unauthorized.shtml</a>	Published 2006		p-RfC	0.06	mg/m3	17		LOAEL	185	mg/m3	3000	x10 inter species, x 10 intra species, x 10 limited study duration x 3 for database limitations

## Trans 1,2 Dichloroethene

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
International Programme on Chemical Safety (IPCS)	Barnes 90 day CD1 mice study using the trans isomer	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Increased serum alkaline phosphate levels in males and decreased thymus weight in females. Human effects include CNS depression, neurological effects and trans is estimated to be 2x more potent than cis isomer	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72) Primary study - Barnes DW et al. 1985. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chemistry and toxicology, 1985, 8:373-407	<a href="http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf</a>
Joint Expert Committee on Food Additives (JECFA)	Barnes 90 day CD1 mice study using the trans isomer	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Increased serum alkaline phosphate levels in males and decreased thymus weight in females. Human effects include CNS depression, neurological effects and trans is estimated to be 2x more potent than cis isomer	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72) Primary study - Barnes DW et al. 1985. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chemistry and toxicology, 1985, 8:373-407	<a href="http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwg/1,2-Dichloroethene.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Barnes 90 day mouse drinking water study	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Increased serum alkaline phosphate levels in males and decreased thymus weight in females.	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001 Primary study - Barnes DW et al. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chemistry and toxicology, 1985, 8:373-407	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Barnes 90 day mouse drinking water study	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Hepatic	ATSDR Minimum Risk Levels December 2008 and Toxicological Profile for 1,2-Dichloroethene, ATSDR, 1996 available at <a href="http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf</a> (Primary Reference for the Study: Barnes, D.W., V.M. Sanders, K.L. White, Jr., et al. 1985. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chem. Toxicol. 8: 373-392.)	<a href="http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf">http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf</a>
USEPA Acute Guideline Levels (AELs)					
USEPA Health Advisors					
USEPA Integrated Risk Information System (IRIS)	Barnes 90 day mouse drinking water study	CD1 Mice received trans-1,2-dichloroethene in drinking water. Dose groups of 17, 175 and 387 mg/kg-bw/day. No effects at 17mg/kg-bw/day	Increased serum alkaline phosphate levels in males and decreased thymus weight in females.	Barnes, D.W., V.M. Sanders, K.L. White, Jr., et al. 1985. Toxicology of trans-1,2-dichloroethylene in the mouse. Drug Chem. Toxicol. 8: 373-392.	<a href="http://toxnet.nlm.nih.gov/cgi-bin/sis/search">http://toxnet.nlm.nih.gov/cgi-bin/sis/search</a>
Toxicology Data Network (Toxnet)	See IRIS above	See IRIS above	See IRIS above	See IRIS above	See IRIS above
TDI inhalation					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	Freundt Semi-chronic inhalation study on Rats	Rats exposed to 780mg/m <sup>3</sup> for 8 hours a day, 5 days a week for 8 or 16 weeks. 780mg/kg equivalent to 185mg/m <sup>3</sup> after adjustment for continuous exposure - this is an LOAEL	Liver (degeneration of liver lobules and Kupffer Cells) and lungs (pulmonary hyperaemia, alveolar septal distention and pneumonic infiltration) were effected	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001 (Primary Study: Freundt et al. 1977. Toxicity Studies on trans-1,2-dichloroethylene. Toxicology 7, 141-153)	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk levels	Freundt Semi-chronic inhalation study on Rats	Rats exposed to 780mg/m <sup>3</sup> for 8 hours a day, 5 days a week for 8 or 16 weeks. 780mg/kg equivalent to 185mg/m <sup>3</sup> after adjustment for continuous exposure - this is an LOAEL	Liver (degeneration of liver lobules and Kupffer Cells) and lungs (pulmonary hyperaemia, alveolar septal distention and pneumonic infiltration) were effected	Primary Study: Freundt et al. 1977. Toxicity Studies on trans-1,2-dichloroethylene. Toxicology 7, 141-153	<a href="http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf">http://www.atsdr.cdc.gov/mrls/pdfs/atsdr_mrls_december_2008.pdf</a>
US EPA Provisional Peer Reviewed Toxicity Values (PPRTV)	Freundt Semi-chronic inhalation study on Rats	Rats exposed to 780mg/m <sup>3</sup> for 8 hours a day, 5 days a week for 8 or 16 weeks. 780mg/m <sup>3</sup> equivalent to 185mg/m <sup>3</sup> after adjustment for continuous exposure - this is an LOAEL	Liver (degeneration of liver lobules and Kupffer Cells) and lungs (pulmonary hyperaemia, alveolar septal distention and pneumonic infiltration) were effected	Provisional Peer Reviewed Toxicity Values for cis-1,2-dichloroethylene, Superfund Health Risk Technical Support Centre for Environmental Assessment, 2006. (Primary Study: Freundt et al. 1977. Toxicity Studies on trans-1,2-dichloroethylene. Toxicology 7, 141-153)	

Trans-1,2-dichloroethene		CAS 156-60-5	Assessor A: Date	Nick Brown Grontmij 29/05/2009	Assessor B Date	Catherine Helm WD Environmental 01/06/2009	Final Review Date	Panel/SF 28/08/2009
MDI			Recommended MDI <sub>oral</sub>	Units	Only US Data has been identified. In the majority of cases exposure through drinking water and food is likely to be negligible however sources in drinking water have been identified. A value of 4ug day <sup>-1</sup> for background exposure through drinking water is tentatively proposed within the WHO Background document for development of WHO Guidelines for Drinking Water Quality. This value appears to be based on the US study that identified detectable concentrations in 8% of drinking water sources with detectable concentrations ranging between 2-120ug/l. In conjunction with the MDI Inhalation (6ug day <sup>-1</sup> see below) this equates to a total of 10ug/day background exposure which conforms reasonably well with the RIVM estimate of total background exposure to the mixed isomers of 0.13ug/kg-bw/day (9.1ug/day for a 70kg adult). The same value has also been selected for the cis isomer since the primary study does not distinguish between the two isomers.			
			4	ug day <sup>-1</sup>				
Organisation	Date	Media	Value	Units	Description	Reference	Web link	
International Programme on Chemical Safety (IPCS)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>	
Joint Expert Committee on Food Additives (JEFCA)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>	
WHO Guidelines for Drinking Water Quality	14/04/2009	Drinking water	4	ug/day	1,2 dichloroethene (mixed isomers) detected in 8% of drinking supplies derived from groundwater, at concentrations between 2-120ug/l. The high end value is therefore greatly atypical with the majority of drinking water containing concentrations less than detection levels. Estimated 4ug/l MDI is based on a concentration of 2ug/l in drinking water.	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Drinking water	0-120	ug/l	Dutch data not available. 1,2 dichloroethene (mixed isomers) detected in 8% of drinking supplies derived from groundwater, at concentrations between 2-120ug/l. RIVM estimated background exposure of 0.13ug/kg-bw/day for the mixed isomers via inhalation and oral intake.	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Drinking water	0-120	ug/l	1,2 dichloroethene (mixed isomers) detected in 8% of drinking supplies derived from groundwater, at concentrations between 2-120ug/l. The high end value is atypical with the majority of drinking water containing concentrations less than detection levels.	Toxicological Profile for 1,2-Dichloroethene, ATSDR, 1996	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf</a>	
USEPA Health Advisories	14/04/2009	DW	0.07	mg/l	MCLG & MCL		<a href="http://www.epa.gov/waterscience/criteria/drinking/">www.epa.gov/waterscience/criteria/drinking/</a>	
Toxicological Data Network (TOXNET)	14/04/2009		ND to 2,277	ug/l	ADI from water in HSDB Database (trans isomer specific)	USEPA: National Contaminant Occurrence Database. trans-1,2-Dichloroethylene. Available from the Database Query page at <a href="http://www.epa.gov/safewater/data/ncod.html">http://www.epa.gov/safewater/data/ncod.html</a> as of Apr 12, 2001.	<a href="http://toxnet.nlm.nih.gov/">http://toxnet.nlm.nih.gov/</a>	
MDI			Recommended MDI <sub>inh</sub>	Units	Only US Data has been identified. The value of 6ug/day is the maximum concentration (for mixed isomers) within range that ATSDR suggest that the general US population is likely to be exposed to. In conjunction with the MDI Oral (4ug day <sup>-1</sup> see below) this equates to a total of 10ug/day background exposure which conforms reasonably well with the RIVM estimate of total background exposure to the mixed isomers of 0.13ug/kg-bw/day (9.1ug/day for a 70kg adult). The same value has also been selected for the Cis isomer since ATSDR do not distinguish between the two isomers.			
			6	ug day <sup>-1</sup>				
Organisation	Date	Media	Value	Units	Description	Reference	Web link	
Joint Expert Committee on Food Additives (JEFCA)	14/04/2009	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	See WHO Guidelines for DWQ	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>	
WHO Guidelines for Drinking Water Quality	14/04/2009	Urban and suburban air	644 (Based on 20m <sup>3</sup> x 32.2ug/m <sup>3</sup> )	ug/day	1,2 Dichloroethene (mixed isomers) recorded at mean concentrations of 32.2ug/m <sup>3</sup> within indoor air (Data source unclear).	WHO (2003) 1,2-Dichloroethene in drinking-water. Background document for preparation of WHO Guidelines for drinking-water quality. Geneva, World Health Organization, (WHO/SDE/WSH/03.04/72)	<a href="http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf">http://www.who.int/water_sanitation_health/dwq/1,2-Dichloroethene.pdf</a>	
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) Levels	14/04/2009	Urban and suburban air	0.27 (Cis isomer) No background concentration is provided for Trans in air	ug/m <sup>3</sup>	Dutch data not available. RIVM estimated background exposure of 0.13ug/kg-bw/day for the mixed isomers via inhalation and oral intake.	RIVM Report 711701 025. Re-evaluation of human toxicological maximum permissible risk levels A.J. Bars, R.M.C Theelan, P.J.C.M. Janssen, J.M. Hesse, M.E. van Apeldoorn, M.C.M. Meijerink, L.Verdam, M.J.Zeilmaker March 2001	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701025.pdf</a>	
US Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles and Minimal Risk Levels	14/04/2009	Ambient air	6	ug/day	The general population (USA) estimated to be exposed to low levels of 1,2 dichloroethene (mixed isomers) through inhalation in urban air (1-6ug/day)	Toxicological Profile for 1,2-Dichloroethene, ATSDR, 1996	<a href="http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf">http://www.atsdr.cdc.gov/toxprofiles/tp87.pdf</a>	

Substance:		Trans 1,2 Dichloroethene		CAS Number:		156-60-5		Assessor A:		Claire Potter		Assessor B:		Catherine Helm		Final Review:		Panel/SF											
Chemical Formula:		C2H2Cl2		Phase at Ambient Temperature:		Liquid		Date:		01-Apr-09		Date:		29/05/2009		Date:		28/08/2009											
Property		Units	Calculated Value	Adopted Value	Ref. Temp (C)	Rationale		References		A		B		C		D		E		F		G		H					
Required Parameters										HOWARD, 1990		LIDE, 2008		MACKAY et al, 2006		MERCCK, 2006		MONTGOMERY, 2007		MONTGOMERY, 1997		NIST, 2005		OECD, 2000					
						Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)	Source Units	SR7 Units	Ref. Temp (C)			
Relative Molecular Mass	g mol <sup>-1</sup>	n/a	96.94	n/a		g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)	g mol <sup>-1</sup>	g mol <sup>-1</sup>	Ref. Temp (C)			
						Average	96.94	96.94	n/a	96.94	96.94	n/a	96.94	96.94	n/a	96.94	96.94	n/a	96.94	96.94	n/a	96.94	96.94	n/a	96.94	96.94	n/a		
Henry's Law Constant (HLC)	Pa m <sup>3</sup> mol <sup>-1</sup>	n/a	9.60E+02	25		atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	KPa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	Pa m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	n/a	n/a	n/a	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	mol kg <sup>-1</sup> bar <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	atm m <sup>3</sup> mol <sup>-1</sup>	Pa m <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
						Geomean	6.72E-03	6.81E+02	25	9.60E-01	9.60E+02	25	8.71E+02	25					Insert Values	25	Insert Values	25	Insert Values	25	1.12E-01	8.96E+02	25	Insert Values	25
Solubility (S) 10 oC where possible. (Use unit converter if source provides different units)	mg/L	n/a	5.25E+03	10		mg/L	mg/L	Ref. Temp (C)	g/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)	mg/L	mg/L	Ref. Temp (C)
						Geomean	6.30E+03	6.30E+03	25	5.30E+00	5300	10	6.26E+03	6.26E+03	25	6.26E+03	6.26E+03	25	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	5.25E+03	5.25E+03	10	Insert Values	Insert Values
Chemical Boiling Point (ambient pressure)	K	n/a	3.21E+02	n/a		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	48	321.15	n/a	48.7	321.85	n/a	48.7	321.85	n/a	47.2	320.35	n/a	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	321	321.00	n/a	Insert Values	Insert Values
Chemical Melting Point (ambient pressure)	K	n/a	2.23E+02	n/a		°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)	°C	K	Ref. Temp (C)
						Average	-50	223.15	n/a	-49.8	223.35	n/a	-49.8	223.35	n/a	-49.4	223.75	n/a	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	223	223.00	n/a	Insert Values	Insert Values
Log Octanol - Water Coefficient	Dimensionless	n/a	2.08E+00	n/a		Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)	Dimensionless	Dimensionless	Ref. Temp (C)
						Average	2.06	2.06	n/a	1.93	1.93	n/a	2.06	2.06	n/a	2.09	2.09	n/a	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	2.09	2.09	n/a	Insert Values	Insert Values
Molar Volume (Le Bas method)	cm <sup>3</sup> mol <sup>-1</sup>	n/a	8.62E+01	n/a		cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)	cm <sup>3</sup> mol <sup>-1</sup>	cm <sup>3</sup> mol <sup>-1</sup>	Ref. Temp (C)
						Average	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Enthalpy of Vaporisation at normal boiling point (EVNBP)	J Mol <sup>-1</sup>	28642.17679	2.86E+04	Normal Chemical Boiling Point	Calculated Value	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)	KJ mol <sup>-1</sup>	J Mol <sup>-1</sup>	Ref. Temp (C)
						Average	28.9	28900	n/a	28.9	28900	n/a	28.9	28900	n/a	28.9	28900	n/a	28.9	28900	n/a	28.9	28900	n/a	28.9	28900	n/a	28.9	28900
Chemical Critical Point temperature (ambient pressure)	K	507.8310394	5.08E+02	n/a	Calculated Value	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)	K	K	Ref. Temp (C)
						Average	n/a	n/a	n/a	516.5	516.50	n/a	n/a	n/a	n/a	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values
Critical Pressure	atm	51.19955043	5.12E+01	None stated	Calculated Value	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)	Bar	Atmosph	Ref. Temp (C)
						Average	n/a	n/a	n/a	55.1	54.379472	n/a	n/a	n/a	n/a	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	Insert Values	

Calculated parameters for input to CLEA model (UPDATED FROM THE SPREADSHEET TOOL)

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Air-water partition coefficient at ambient soil temperature	cm <sup>3</sup> cm <sup>-3</sup>	1.769E-01	10	Estimated from parameters above using Clapyron relationship or direct calculation

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Vapour pressure at ambient soil temperature	Pa	22569.7142	10	Estimated from parameters above using Grain-Watson method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in air	m <sup>2</sup> s <sup>-1</sup>	9.09E-06	10	Estimated from parameters above using Wilkie-Lee method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Diffusion coefficient in water	m <sup>2</sup> s <sup>-1</sup>	7.08E-10	10	Estimated from parameters above using Hayduk and Laudie method

Property	Units	Calculated Value	Ref. Temp (C)	Rationale
Organic carbon-water partition coefficient	Log cm <sup>3</sup> g <sup>-1</sup>	1.78	n/a	Estimated from parameters above using equation in Table 2.12 of SR7

Tributyltin (oxide)	CAS Number:	56-35-9	Assessor A:	Andreas Neymeyer, Buro Happold	Assessor B:	Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF
	Date	16/04/2009	Date	16/04/2009	Date	28/08/2009		

	Oral	Dermal	Inhalation	Combine Oral and Inhalation TDIs	Justification
Apply TDloral to exposure routes?	Yes	Yes	No	Yes	The weight of evidence shows that TBTO is not genotoxic
Apply IDoral to exposure routes?	No	No	No		
Apply TDlinh to exposure routes?	No	No	Yes		
Apply IDinh to exposure routes?	No	No	No		

TDI oral	Recommended TDloral	Units	Justification
	0.25	ug.kg-1.d-1	Consistent value from IPCS, SCF, WHO & RIVM

Organisation	Web Link	Last Updated	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
Scientific Committee on Food (SCF) pre 2002	<a href="http://ec.europa.eu/food/fs/sc/scf/index_en.html">http://ec.europa.eu/food/fs/sc/scf/index_en.html</a>	09/04/2009	27/03/2009	TDI	0.0003	mg/kg body weight per day	0.3		NOAEL	0.025	mg/kg body weight per day		
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	09/04/2009	27/03/2009	TDI	0.0003	mg/kg body weight per day	0.3		NOAEL	0.025	mg/kg body weight per day	100	
		09/04/2009	27/03/2009	TDI	0.0003	mg/kg body weight per day	0.3		NOAEL	0.025	mg/kg body weight per day	100	
WHO Guidelines for drinking water Quality	<a href="http://www.who.int/water_sanitation_health/dwg/guidelines/en">http://www.who.int/water_sanitation_health/dwg/guidelines/en</a>	09/04/2009	27/03/2009	TDI	0.25	ug/kg body weight per day	0.25		NOAEL	0.025	mg/kg body weight per day	100	for inter- and intraspecies variation
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Entrez PubMed	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a> <a href="http://www.ncbi.nlm.nih.gov/entrez/query.fcgi">http://www.ncbi.nlm.nih.gov/entrez/query.fcgi</a>	//2009	28/08/2009	TDI	0.25	ug/kg body weight per day	0.25	medium	NOAEL	0.025	mg/kg body weight per day	100	for inter- and intraspecies variation
		27/03/2009	27/03/2009	TDI	0.25	ug/kg body weight per day	0.25		NOAEL	0.025	mg/kg body weight per day		

TDI inhal	Recommended TDlinhal	Units	Justification
	0.0057	ug.kg-1.d-1	Based on provisional TCA derived by RIVM (0.02 ug/m3 x 20 m3/d /70 kg)

Organisation	Web Link	Date Web Checked	Date Web Checked	Health criteria type	Value	Initial Units	CLEA units ug.kg-1.d-1	Confidence rating	Basis	Value	Units	UF	UF description
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>								No adequate data available to derive a guidance value for inhalation exposure.				
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	<a href="http://www.rivm.nl/en/">http://www.rivm.nl/en/</a>	//2009	28/08/2009	pTCA	0.02	ug/m3	0.0057	provisional value	NAOEL (adjusted)	20	ug/m3	1000	no data

ID oral	Recommended IDoral	Units	Justification
	n/a		The weight of evidence shows that TBTO is not genotoxic

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	09/04/2009	27/03/2009		The weight of evidence shows that TBTO is not genotoxic					

ID inhal	Recommended IDinhal	Units	Justification
	n/a		The weight of evidence shows that TBTO is not genotoxic

Organisation	Web Link	Last Updated	Date Web Checked	Non threshold effects?	Basis	Health criteria type	Value	Units	Confidence rating	Basis
International Programme on Chemical Safety (IPCS)	<a href="http://www.who.int/ipcs/en/">http://www.who.int/ipcs/en/</a>	09/04/2009	27/03/2009		The weight of evidence shows that TBTO is not genotoxic					

## Tributyltin (oxide)

TDI oral					
Organisation	Study type	Description	Target organ/Critical Effect	Reference	Web link
Scientific Committee on Food (SCF) pre 2002	animal (rats)	Long-term animal study with rats	Effects on liver the haematological and the endocrine system	IPCS, 1990.	<a href="http://ec.europa.eu/research/endocrine/pdf/drinking_water_en.pdf">http://ec.europa.eu/research/endocrine/pdf/drinking_water_en.pdf</a>
International Programme on Chemical Safety (IPCS)	animal (rats)	Numerous studies, both short term and long term	Transient increase in adrenal weight shortly after exposure and a transient effect on thyroid follicles. In addition, reversible effects on the pituitary and on levels of adrenocorticotrophic hormones, thyroid-stimulating hormone, thyroxine, and serum cortisol. At the highest dose mortality 5/10 in males and 6/10 in females inflammatory reactions	e.g., Funahashi et al., 1980 Truhaut et al. 1979 Schweinfurth & Gunzel 1987	<a href="http://www.inchem.org/documents/cicads/cicads/cicad14.htm">http://www.inchem.org/documents/cicads/cicads/cicad14.htm</a>
	animal (rats)	"Numerous well-conducted studies, both short term and long term"			<a href="http://www.who.int/ipcs/publications/cicad/en/cicad14.pdf">http://www.who.int/ipcs/publications/cicad/en/cicad14.pdf</a>
WHO Guidelines for drinking water Quality	animal (rats)	17-month feeding study in rats	The most sensitive end-point appears to be immunotoxicity related to suppression of resistance to the nematode <i>Trichinella spiralis</i>		<a href="http://www.emro.who.int/ceha/pdf/Guidelines_DrinkingWater_Recommendations.pdf">http://www.emro.who.int/ceha/pdf/Guidelines_DrinkingWater_Recommendations.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Entrez PubMed	animal (rats)	17-month feeding study in rats	Immunotoxic effects	Vos et al., 1990; Wester et al., 1988, 1990; Tryphonas et al., 2004	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701092.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701092.pdf</a> <a href="http://www.ncbi.nlm.nih.gov/pubmed/18979060?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum">http://www.ncbi.nlm.nih.gov/pubmed/18979060?ordinalpos=1&amp;itool=EntrezSystem2.PEntrez.Pubmed.Pubmed_ResultsPanel.Pubmed_DefaultReportPanel.Pubmed_RVDocSum</a>
TDI inhal					
Organisation	Study type	Description	Response	Reference	Web link
International Programme on Chemical Safety (IPCS)					<a href="http://www.who.int/ipcs/publications/cicad/en/cicad14.pdf">http://www.who.int/ipcs/publications/cicad/en/cicad14.pdf</a>
Dutch National Institute for Public Health and the Environment (RIVM) Maximum Permissible Risk (MPR) levels	animal (rats)	4 week study with rats. Note the provisional TCA is unchanged since first RIVM evaluation of TBTO in 1995. RIVM note that there has been no additional relevant toxicological data in the intervening period.	No data	Janssen PJCM, Apeldoorn ME van, Kolen-Vermeulen JEM van, Mennes WC (1995). Human-Toxicological Criteria for Serious Soil Contamination: Compounds evaluated in 1993 & 1994. RIVM report no. 715810 009. Evaluation of TCA for TBTO based on toxicological study reported by Prins and Van Velzen, 1983 and BUA, 1988	<a href="http://www.rivm.nl/bibliotheek/rapporten/711701092.pdf">http://www.rivm.nl/bibliotheek/rapporten/711701092.pdf</a>
ID oral					
Organisation	Study type	Description	Response	Reference	Web link
International Programme on Chemical Safety (IPCS)					<a href="http://www.inchem.org/documents/cicads/cicads/cicad14.htm">http://www.inchem.org/documents/cicads/cicads/cicad14.htm</a>
ID inhal					
Organisation	Study type	Description	Response	Reference	Web link
International Programme on Chemical Safety (IPCS)					<a href="http://www.inchem.org/documents/cicads/cicads/cicad14.htm">http://www.inchem.org/documents/cicads/cicads/cicad14.htm</a>

Tributyltin (oxide)	CAS 56-35-9	Assessor A: Andreas Neymeyer, Buro Happold	Assessor B: Mike Rogers, OPUS JOYNES PIKE Ltd	Final review:	Panel/SF	
	Date	09/04/2009	Date	09/04/2009	Date	28/08/2009

MDI			Recommended MDI <sub>oral</sub>	Units	Justification: As reported by Tsuda T, Inoue DT, Kojima M, Aoki S (1995)		
Organisation	Date	Media	Value	Units	Description	Reference	Web link
Food Standards Agency	27/03/2009		<8.8 [combined TBT, DBT and TPT intake (average adult consumer)]	ug day-1	"Intake estimates of organotins measured in shellfish in this survey show that the maximum levels found would contribute less than half of the Tolerable Daily Intake (TDI), as set by the European Food Safety Authority (EFSA), for an average adult consumer."  <0.25ug/kg(bw)/day x 70kg(bw)=<17.5ug/day/2=<8.8ug/kg	Food Standards Agency. 2005. SURVEY OF ORGANOTINS IN SHELLFISH (http://www.food.gov.uk/multimedia/pdfs/fsis8105.pdf)	<a href="http://www.food.gov.uk">www.food.gov.uk</a>
European Food Safety Authority (EFSA)	27/03/2009	food	5.8 [combined TBT, DBT and TPT intake (based on mean)]	ug day-1	"Intake calculations based on fish and seafood consumption in Norway, taken as paradigm of high consumption in Europe showed that the combined TBT, DBT and TPT intake estimated from median concentration was 0.018 µg/kg b.w./day (approximately 7 % of the proposed group TDI). The same intake calculated on mean basis was 0.083 µg/kg b.w./day (about 33 % of the proposed group TDI). The intakes for high consumers, calculated on median and mean concentrations were 0.037 and 0.17 µg/kg b.w./day, respectively, which represents approximately 15 % and 70 % of the group TDI."  0.083ug/kg (bw)/day x 70kg (bw) = 5.8ug /day (mean) 0.17ug/kg (bw)/day x 70kg (bw) = 12ug /day [high consumer (mean)]	The EFSA Journal (2004) 102, 1-119 (http://www.efsa.europa.eu/cs/BlobServer/Scientific_Opinion/contam_opinion10_ej102_organotins_v2_en1.pdf?ssbinary=true)	<a href="http://www.efsa.europa.eu/en.htm">www.efsa.europa.eu/en.htm</a>
International Programme on Chemical Safety (IPCS)	27/03/2009	food	9	ug day-1	"Information on tributyltin concentrations in various media that are relevant to estimation of human exposure is extremely limited, being restricted to data from Japan." ... "Tsuda et al. (1995) investigated the daily intakes of tributyltin compounds from meals in Shiga Prefecture, Japan. Daily intakes of TBTO determined by the duplicate-portion method were 4.7 + 7.0 µg/day in 1991 ( n = 39) and 2.2 + 2.2 µg/day in 1992 ( n = 40). Using the market basket method, the daily intake was estimated at 6-9 µg/day in 1991 and 6-7 µg/day in 1992. The TBTO was found mostly in seafood."	Tsuda T, Inoue DT, Kojima M, Aoki S (1995) Daily intakes of tributyltin and triphenyltin compounds from meals. Journal of the Association of Official Analytical Chemists International, 78:941-943 (http://www.inchem.org/documents/cicads/cicads/cicad14.htm)	<a href="http://www.who.int/ipcs/en">www.who.int/ipcs/en</a>
MDI			Recommended MDI <sub>inh</sub>	Units	Justification: No suitable data for background exposure available - background exposure from inhalation of TBTO is assumed to be negligible		
			0	ug day-1			
Organisation	Date	Media	Value	Units	Description	Reference	Web link

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### 3.54 Tributyl tin oxide

Tributyl tin oxide, TBTO, or hexabutyldistannoxane (CAS No. 56-35-9) is an effective **biocide** preservative for wood, cotton textiles, paper, and paints for residential homes (IPCS 1999). It is an **antifouling agent** in numerous formulations of marine paints as an organometallic copolymer (IPCS 1999). It is a low volatile, flammable liquid at room temperature (IPCS 1999). The recommended physical-chemical data for the derivation of Soil Guideline Values is shown in Table 3.54.

**Table 3.54 Physical-chemical data for tributyl tin oxide**

Chemical Property		Comments
Data required for CLEA software	At 10°C unless stated	
Air-water partition coefficient ( $K_{aw}$ )	4.24E-05	Estimated by Clapeyron relationship from the Henry's law constant at 25°C
Diffusion coefficient in air	3.25E-06 m <sup>2</sup> s <sup>-1</sup>	Estimated by Wilke and Lee method
Diffusion coefficient in water	2.49E-10 m <sup>2</sup> s <sup>-1</sup>	Estimated by Hayduk and Laudie method
Log (Octanol-water partition coefficient) ( $K_{ow}$ )	4.05	Estimated by KOWWIN method
Log (Organic carbon-water partition coefficient) ( $K_{oc}$ )	3.13 cm <sup>3</sup> g <sup>-1</sup>	Estimated by linear regression from log $K_{ow}$
Molecular weight	596.11 g mol <sup>-1</sup>	Recommended literature value
Vapour pressure	8.56E-04 Pa	Estimated by Grain-Watson method
Water solubility	5.1 mg L <sup>-1</sup> (25°C)	Estimated by WSKOWIN method
<b>Other useful data</b>		
Chemical formula	C <sub>24</sub> H <sub>54</sub> OSn <sub>2</sub>	
Boiling point	654.9 K	Estimated by Banks method
Critical point temperature	982.4 K	Estimated by Guldberg approximation method
Enthalpy of vaporisation at boiling point	62,867 J mol <sup>-1</sup>	Estimated by Fishtine method
Henry's law constant	6.01E-01 Pa m <sup>3</sup> mol <sup>-1</sup> (25°C)	Estimated by direct calculation at 25°C
Melting point	228.2 K	Recommended literature value
Physical state at room temperature	Liquid	





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