

Final report

## S-Risk for the Walloon region - substance data sheets part 3: Chloroaliphatic substances, chlorobenzenes and chlorophenols

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**LIST OF ACRONYMS**

ABS	Absorption factor
Al	Aluminum content
BCF	Bioconcentration factor
BTEXS	benzene, toluene, ethylbenzene, styrene
BTF	Biotransfer factor
Da	Diffusion coefficient in air
Dpe	Diffusion coefficient in polyethylene
Dpvc	Diffusion coefficient in PVC
Dw	Diffusion coefficient in water
FA	Factor used when calculating dermal absorption from water
Fe	Iron content
ISSeP	Institut Scientifique de Service Public
$K_d$	Sorption coefficient soil-water
Koa	Distribution coefficient octanol-air
Koc	Distribution coefficient organic carbon-water
Kow	Distribution coefficient octanol-water
Kp	Dermal permeability coefficient
MTBE	methyl-t-butylether
OVAM	Openbare Vlaamse Afvalstoffenmaatschappij (Public Waste Agency of Flanders)
PAK	polycyclic aromatic hydrocarbons
Ptot	Total phosphorus content
TCL	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document

## LIST OF MODIFICATIONS

<b>Date</b>	<b>Modification</b>
16/11/2017	Removal of concentration limits for 1,2-dichloroethane and pentachlorophenol in plants and animal products.
29/03/2018	Modification of some toxicological threshold values for hexachlorobenzene (TDI, TDU and TCA), pentachlorobenzene (TCA) and 2,3,4,6 tetrachlorophenol (TCA).

## INTRODUCTION

The **substance data sheets** summarise the data as available in S-Risk 1.0 for the **Walloon region**. The substance data sheets are a copy of those used for the S-Risk Flanders version. They are not based on the Annexe B4 (“propriétés physico-chimiques de référence pour les polluants normés”) of the GRER part B version 2.0. The differences between the Flemish and Walloon Region are highlighted using **W** (representing data used only in the Walloon version). Physiological parameters and BCF/BTF are the same for the two regions. The three main differences are:

- Toxicological values (values recently revised and harmonized in Wallonia);
- Carcinogenicity revision;
- Limit values used in Wallonia are regulatory values only (“code de l’eau” for drinking water and AGW, 2010 and EC, 2004 for outdoor air). No limit values in indoor air nor in plants and meats are proposed.
- All background values are set to “0” (background values are not taken into account in Wallonia).

Substance data sheets modified for the Walloon version summarize the data as available in S-Risk 1.0 for the Walloon region.

The current **substance data sheets** used for the **Flanders version** of S-Risk are a copy of those used for the calculation of the proposed soil clean-up values in Flanders, with some modifications. Following changes in model equations in S-Risk compared to the formerly used Vlier-Humaan model, some new parameter values had to be introduced. Also some supplementary options available in S-Risk required changes to the input data for which new values had to be collected. The most important changes are:

- **Dermal absorption:** Two new parameters are used that replace the formerly used parameters to calculate dermal absorption, namely the fraction adsorbed for dermal uptake via soil and dust, and the dermal permeability coefficient for dermal uptake from water. The latter parameter is combined with a parameter FA.
- **Bioconcentration factors plants (BCF):** For metals and arsenic very often either the BCF for maize or the BCF for grass was missing. In these cases the same BCF was used for maize and grass. Because this is incorrect, there is a need to search for additional BCFs.
- **Bioconcentration factors plants (BCF):** for organic compounds plant uptake in S-Risk can either be calculated starting from substance- and plant-specific characteristics or directly from BCF values expressed in mg/kg dm in the plant per mg/m<sup>3</sup> soil solution. For most organic substances plant uptake is calculated. For some organic substances however, BCF values reported in the original (Vlier-Humaan) data sheets had units of mg/kg dm in the plant per mg/kg dm in the soil, which are incompatible with the current S-Risk version. For these substances plant- and substance specific characteristics were used to calculate plant uptake. If so, this is mentioned in the data sheets.
- **Biotransfer factors animal products (BTF):** S-Risk allows to specify BTF animal products by meat, milk, kidney and liver. For inorganic substances BTF values need to be filled in. The original data sheets only provided values for meat and milk. Lacking values were collected from De Raeymaecker et al. (2005). For organic substances model calculations are always used to obtain BTF values.
- **Biotransfer factors eggs (BTF):** S-Risk allows the user to calculate transfer to chicken eggs. This is a new feature as compared to Vlier-Humaan. However, using default settings in S-Risk this exposure route is not activated. For metals biotransfer factors to eggs have been collected and are included in the substance data sheets. For organic substances no BTF

have been collected and their value has been equaled to zero. When the exposure route to eggs is activated in S-Risk the user should enter appropriate BTF values.

- **Toxicity data:** The toxicity data in S-Risk are copied from the original substance data sheets. In contrast to Vlier-Humaan, where calculations were only possible for systemic effects and either carcinogenic or non-carcinogenic effects, S-Risk allows to make calculations for several endpoints simultaneously. As a consequence, the toxicity data in the current substance data sheets are sometimes more extensive than in the former ones.
- **Background exposure and background concentrations:** Vlier-Humaan did only allow to enter one value for background exposure (be it depending on the type of land use) via food. In S-Risk it is possible to enter age-dependent background exposure via food. Default ratios are most often used for age-dependency (according to the ratios specified in the TGD). Differences between land-uses are taken into account based on the background concentrations for food that have been entered. S-Risk also separately calculates background exposure via drinking water.
- **Limit values for food:** For some substances calculated concentrations in food stuffs have to comply with existing standards. With this in mind recent legislation has been scrutinised and obsolete values were replaced by more recent ones when appropriate.

The existing information, which was copied in S-Risk is based on the following original substance data sheets:

- Heavy metals: OVAM (2009c) and (OVAM, 2009d) with accompanying spreadsheet;
- BTEXS: OVAM (2009a);
- Chlorinated aliphatic substances: OVAM (2004) for 1,1,1-trichloroethane, 1,1,2-trichloroethane, 1,1-dichloroethane, cis-1,2-dichloroethene, trans-1,2-dichloroethene, dichloromethane, tetrachloroethene, tetrachloromethane, trichloroethene; OVAM (2009b) for 1,2-dichloroethane, vinyl chloride, trichloromethane (chloroform);
- Chloro-aromatics: OVAM (2004); OVAM (2009b) for hexachloro-benzene;
- PAHs: OVAM (2003a) for PAHs; OVAM (2005a) for changes in the evaluation criteria for benzo(a)pyrene and dibenzo(a,h)anthracene;
- Cyanides: OVAM (2004);
- Trimethylbenzenes: OVAM (2003b);
- Chlorophenols: OVAM (2005b)
- Hexane, heptane, octane: OVAM (2004);
- MTBE: OVAM (2003a)

Details on the new information are always available in the report discussing the calculation of clean-up values with S-Risk (Cornelis, Standaert, and Willems, 2013). Newly added or modified information compared to the original data sheets is clearly indicated in the S-Risk substance data sheets.

Changes entered after publication of the first version of the substance datasheets are listed in the section "List of modifications".

The substance data sheets consist of 6 documents:

- Part 1: Substance data sheets metals and arsenic
- Part 2: Substance data sheets benzene, toluene, ethylbenzene, xylenes, styrene, phenol and trimethylbenzenes
- **Part 3: Substance data sheets chlorinated aliphatic substances, chloro benzenes and chlorophenols**



- Part 4: Substance data sheets polycyclic aromatic hydrocarbons
- Part 5: Substance data sheets alkanes, MTBE and cyanides
- Part 6: Substance data sheets total petroleum hydrocarbons

## CHAPTER 4. SUBSTANCE DATA SHEETS CHLORINATED ALIPHATIC SUBSTANCES

Data on substances that do not derive from the former substance data sheets are indicated with **N**, accompanied with some explanation if appropriate. Detailed information on all new entries is given in Cornelis et al. (2013). Data on substances that differ from Flanders are indicated with **W**. Volatile pollutants (vapour pressure > 0.1Pa at 20°C) are highlighted in the document.

As the chlorinated aliphatics have been assessed in multiple background documents, the applicable report by chemical is listed below.

Chemical name	Report
Dichloromethane*	Cornelis and Geuzens (1995)
Tetrachloromethane*	Cornelis and Geuzens (1995)
Tetrachloroethylene*	Cornelis and Geuzens (1995)
Trichloroethylene*	Cornelis and Geuzens (1995)
1,1,1-trichloroethane*	Nouwen and Cornelis (1998)
1,1,2-trichloroethane	Nouwen and Cornelis (1998)
1,1-dichloroethane	Nouwen and Cornelis (1998)
c-1,2-dichloroethene	Nouwen and Cornelis (1998)
t-1,2-dichloroethene	Nouwen and Cornelis (1998)
1,2-dichloroethane**	De Raeymaecker et al. (2003)
vinylchloride	De Raeymaecker et al. (2003)
trichloromethane	De Raeymaecker et al. (2003)

\*: toxicology under review

\*\* : important remarks given in the substance data sheet

## 4.1. DICHLOROMETHANE

Parameter	Unit	Value	Source
CAS nr.		75-09-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	85	
Solubility	mg/l	$1.99 \times 10^4$ (25°C)	Kühne et al. (1995)
Vapour pressure*	Pa	46518 (20°C)	Verschueren (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	116 (10°C)	Gosset (1987); Wright et al. (1992); Tse en Sandler (1992)
log Kow	g/g	1.48	van den Berg (1994); US-EPA (1994)
log Koc	dm <sup>3</sup> /kg	1.361728	US-EPA (1994)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$5 \times 10^{-7}$	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2A Likely to be carcinogenic to humans	W IARC (2015) W US-EPA (2011a)
Systemic effects threshold			
TDI oral	mg/kg.d	$6.0 \times 10^{-2}$	W ATSDR (2000); Baars, et al. (2001); Health Canada (1996)
TCL inhalation	mg/m <sup>3</sup>	$4.4 \times 10^{-2}$	W Ontario (2008)
TDI dermal	mg/kg.d	$6.0 \times 10^{-2}$	W = oral TDI
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	$7.5 \times 10^{-3}$	W US-EPA (1995a)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	$4.7 \times 10^{-4}$	W US-EPA (1995a)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	$7.5 \times 10^{-3}$	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	

Parameter	Unit	Value	Source
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.2. TETRACHLOROMETHANE

Parameter	Unit	Value	Source
CAS nr.		56-23-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	154	
Solubility	mg/l	800 (20°C)	Verschueren (1983), Broholm en Feenstra (1995), Tse en Sandler (1992), Wright et al. (1992)
Vapour pressure*	Pa	12000 (20°C)	van den Berg (1994)
Henry coefficient	Pa m <sup>3</sup> /mol	1350 (10°C)	Gosset (1987), Tse en Sandler (1992)
log Kow	g/g	2.7	US-EPA (1994)
log Koc	dm <sup>3</sup> /kg	2.22 (Koc = 164)	US-EPA (1994), Kile et al. (1995)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	8x10 <sup>-7</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2B Likely to be carcinogenic to humans	W IARC (1999b) W US-EPA (2010b)
Systemic effects threshold			
TDI oral	mg/kg.d	4.0x10 <sup>-3</sup>	W US-EPA (2010)
TCL inhalation	mg/m <sup>3</sup>	2.4x10 <sup>-3</sup>	W Ontario (2008)
TDI dermal	mg/kg.d	4.0x10 <sup>-3</sup>	W = oral TDI
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	1.0x10 <sup>-8</sup>	W dummy value (considered non-carcinogenic by oral exposure)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	6.0x10 <sup>-3</sup>	W US-EPA (2010)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	1.0x10 <sup>-8</sup>	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	

Parameter	Unit	Value	Source
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.3. TETRACHLOROETHYLENE

Parameter	Unit	Value	Source
CAS nr.		127-18-4	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	165.8	
Solubility	mg/l	$1.50 \times 10^2$ (25°C)	Verschuieren (1983)
Vapour pressure*	Pa	2483 (25°C)	Verschuieren (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	733 (10°C)	Gosset (1987)
log Kow	g/g	2.74	Verschuieren (1983), Mackay (1982)
log Koc	dm <sup>3</sup> /kg	2.421604	US-EPA (1994)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$7.7 \times 10^{-7}$	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	$1.41 \times 10^{-1}$	N Frasch en Barbero (2009)
FA	-	1	N
ABS dermal soil/dust	-	$3.00 \times 10^{-2}$	N US-EPA (1995b, 2003)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2A B1 2	W IARC (1979) W US-EPA (2012) W EC (1996)
Systemic effects threshold			
TDI oral	mg/kg.d	$6.0 \times 10^{-3}$	W US-EPA (2012)
TCL inhalation	mg/m <sup>3</sup>	$4.1 \times 10^{-2}$	W ATSDR (2014)
TDI dermal	mg/kg.d	$6.0 \times 10^{-3}$	W = oral TDI
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	$2.1 \times 10^{-3}$	W US-EPA (2012)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	$5.9 \times 10^{-3}$	W OEHHA (1991)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	$2.1 \times 10^{-3}$	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	4	W AGW (2016)
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	

Parameter	Unit	Value	Source
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg.day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)



## 4.4. TRICHLOROETHYLENE

Parameter	Unit	Value	Source
CAS nr.		79-01-6	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	131.5	
Solubility	mg/l	1.40x10 <sup>3</sup> (20°C)	Tse en Sandler (1992), Wright et al. (1992)
Vapour pressure*	Pa	8000 (20°C)	Verschueren (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	419 (10°C)	Gosset (1987), Tse en Sandler (1992), Wright et al. (1992)
log Kow	g/g	2.4	US-EPA
log Koc	dm <sup>3</sup> /kg	1.939519	US-EPA
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	1.60x10 <sup>-6</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	1.20x10 <sup>-1</sup>	N Nakai et al. (1999)
FA	-	1	N
ABS dermal soil/dust	-	5.90x10 <sup>-3</sup>	N derived from Poet et al. (2000) en Spalt et al. (2009)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		1 A 2	W IARC (2014) W US-EPA (2011b) W EC (2001)
Systemic effects threshold			
TDI oral	mg/kg.d	5.0x10 <sup>-4</sup>	W ATSDR (2014); US-EPA (2011b)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-3</sup>	W ATSDR (2014); US-EPA (2011b)
TDI dermal	mg/kg.d	5.0x10 <sup>-4</sup>	W = oral TDI
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	8.11x10 <sup>-4</sup>	W Santé Canada (2005)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	5.0x10 <sup>-3</sup>	W US-EPA (2011b)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	8.11x10 <sup>-4</sup>	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	7	W AGW (2016)
Limit value in plants	mg/kg fw	-	

Parameter	Unit	Value	Source
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.5. 1,1,1-TRICHLOROETHANE

Parameter	Unit	Value	Source
CAS nr.		71-55-6	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	133.41	Verschueren (1996)
Solubility	mg/l	1.02x10 <sup>3</sup> (20°C)	average of 6 data points
Vapour pressure*	Pa	14346 (20°C)	average of 6 data points
Henry coefficient	Pa m <sup>3</sup> /mol	726 (10°C)	regression based on 23 measurements
log Kow	g/g	2.45	average of 12 data points
log Koc	dm <sup>3</sup> /kg	2.01	average of 8 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	2.00x10 <sup>-6</sup>	Kreule et al. (1995)
Dpvc	m <sup>2</sup> /d	2.00x10 <sup>-9</sup>	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	1.67x10 <sup>-1</sup>	N Fan et al. (2007)
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		3	IARC (1999b)
Systemic effects threshold			
TDI oral	mg/kg.d	2.0	US-EPA (2007)
TCL inhalation	mg/m <sup>3</sup>	2.5x10 <sup>-1</sup>	Hassauer et al. (1993)
TDI dermal	mg/kg.d	2.0	W = oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W

Parameter	Unit	Value	Source
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.6. 1,1,2-TRICHLOROETHANE

Parameter	Unit	Value	Source
CAS nr.		79-00-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	133.41	Verschueren (1996)
Solubility	mg/l	4.44x10 <sup>3</sup> (20°C)	average of 4 data points
Vapour pressure*	Pa	2533 (20°C)	average of 6 measurements
Henry coefficient	Pa m <sup>3</sup> /mol	80 (10°C)	Average of 4 measurements
log Kow	g/g	2.1	average of 6 data points
log Koc	dm <sup>3</sup> /kg	1.8	average of 12 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	2.00x10 <sup>-6</sup>	= value 1,1,1-trichloroethane
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	8.40x10 <sup>-2</sup>	N value in Fan et al. (2007) for 1,1,1-trichloroethane, divided by 2
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		3	IARC (1999b)
Systemic effects threshold			
TDI oral	mg/kg.d	4x10 <sup>-3</sup>	US-EPA (1987a)
TCL inhalation	mg/m <sup>3</sup>	3.9x10 <sup>-2</sup>	Hassauer et al. (1993)
TDI dermal	mg/kg.d	4x10 <sup>-3</sup>	= oral value
averaging period		child, adolescent, adult	
Systemic effects non-threshold			W
Oral slope factor	(mg/kg.d) <sup>-1</sup>	7.2x10 <sup>-2</sup>	W OEHHA (2009)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	1.6x10 <sup>-2</sup>	W US-EPA (1987a)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	7.2x10 <sup>-2</sup>	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	

Parameter	Unit	Value	Source
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	N no values

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.7. 1,1-DICHLOROETHANE

Parameter	Unit	Value	Source
CAS nr.		75-34-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	98.96	Verschueren (1996)
Solubility	mg/l	$5.40 \times 10^3$ (20°C)	average of 5 data points
Vapour pressure*	Pa	25771 (20°C)	regression on 13 data
Henry coefficient	Pa m <sup>3</sup> /mol	249 (10°C)	regression on 15 data
log Kow	g/g	1.79	average of 7 data points
log Koc	dm <sup>3</sup> /kg	1.55	average of 6 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$3.00 \times 10^{-7}$	Kreule et al (1995)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	$2.59 \times 10^{-1}$	N = value 1,2-dichloroethane
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		C	W US-EPA (1996a)
Systemic effects non-threshold			W
Oral slope factor	(mg/kg.d) <sup>-1</sup>	$5.7 \times 10^{-3}$	W OEHA (2009)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	$1.6 \times 10^{-3}$	W OEHA (1999a)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	$5.7 \times 10^{-3}$	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	

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Parameter	Unit	Value	Source
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)



## 4.8. 1,2-DICHLOROETHANE

Parameter	Unit	Value	Source
CAS nr.		107-06-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	98.97	Geometric mean
Solubility	mg/l	8.59x10 <sup>3</sup> (20°C)	Geometric mean
Vapour pressure*	Pa	8528 (20°C)	Geometric mean
Henry coefficient	Pa m <sup>3</sup> /mol	98.23 (20°C)	calculated
log Kow	g/g	1.52	Geometric mean
log Koc	dm <sup>3</sup> /kg	1.418798	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	3.00x10 <sup>-7</sup>	Van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.888	US-EPA (1996c)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	8.64x10 <sup>-5</sup>	US-EPA (1996c)
Kp	[cm/h]	2.59x10 <sup>-1</sup>	N Frasch and Barbero (2009)
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2B B2	IARC (1999b) US-EPA (2001)
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	1.19x10 <sup>-2</sup>	W Derived from inhalation
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	2.6x10 <sup>-2</sup>	W US-EPA (1987b)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	1.19x10 <sup>-2</sup>	W = oral value
Limit in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	3	W EC (1998); Code de l'Eau (2004)
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	

Parameter	Unit	Value	Source
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	W

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.9. CIS-1,2-DICHLOROETHYLENE

Parameter	Unit	Value	Source
CAS nr.		156-59-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	96.95	
Solubility	mg/l	800 (20°C)	Average of 2 data points
Vapour pressure*	Pa	20990 (20°C)	Regression on 9 data
Henry coefficient	Pa m <sup>3</sup> /mol	226 (10°C)	regression on 8 data
log Kow	g/g	1.14	average of 4 data points
log Koc	dm <sup>3</sup> /kg	1.67	average of 4 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	4.00x10 <sup>-8</sup>	Kreule et al. (1995)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		D	US-EPA (2010)
Systemic effects threshold			
TDI oral	mg/kg.d	1.7x10 <sup>-2</sup>	WHO (2008)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-3</sup>	W Québec (2002)
TDI dermal	mg/kg.d	1.7x10 <sup>-2</sup>	= oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	

Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.10. TRANS-1,2-DICHLOROETHYLENE

Parameter	Unit	Value	Source
CAS nr.		156-60-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	96.95	
Solubility	mg/l	600 (20°C)	average of 2 data points
Vapour pressure*	Pa	34438 (20°C)	regression on 9 data
Henry coefficient	Pa m <sup>3</sup> /mol	449 (10°C)	regression on 11 data
log Kow	g/g	1.41	average of 3 data points
log Koc	dm <sup>3</sup> /kg	1.68	average of 3 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	4.00x10 <sup>-8</sup>	Kreule et al (1995)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		D	US-EPA (2010c)
Systemic effects threshold			
TDI oral	mg/kg.d	1.7x10 <sup>-2</sup>	WHO (2008)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-3</sup>	W Québec (2002)
TDI dermal	mg/kg.d	1.7x10 <sup>-2</sup>	= oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/kg fw	-	
Limit value in plants			
Limit value in meat	mg/kg fw	-	
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	

Parameter	Unit	Value	Source
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 4.11. VINYLCHLORIDE

Parameter	Unit	Value	Source
CAS nr.		75-01-1	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	62.5	Geometric mean
Solubility	mg/l	1116 (20°C)	Geometric mean
Vapour pressure*	Pa	332678 (20°C)	Geometric mean
Henry coefficient	Pa m <sup>3</sup> /mol	18637 (20°C)	Calculated
log Kow	g/g	1.24	Geometric mean
log Koc	dm <sup>3</sup> /kg	1.080987	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	3.00x10 <sup>-7</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.912 (25°C)	US-EPA (1996c)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	1.06E-05 (25°C)	US-EPA (1996c)
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		1 A 1	IARC (2012) US-EPA (2000) W EC (1993)
Systemic effects threshold			
TDI oral	mg/kg.d	3x10 <sup>-3</sup>	ATSDR (2006b)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-4</sup>	W Ontario (2008)
TDI dermal	mg/kg.d	3x10 <sup>-3</sup>	= oral value
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	1.5	W US-EPA (2000)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	1.77x10 <sup>-2</sup>	W OEHHA (1990); Québec (2002) mean value
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	1.5	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	0.5	W EC (1998); Code de l'Eau (2004)
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	

Parameter	Unit	Value	Source
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	W

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)



## 4.12. TRICHLOROMETHANE

Parameter	Unit	Value	Source
CAS nr.		67-66-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	119.39	Geometric mean
Solubility	mg/l	8100 (20°C)	Geometric mean
Vapour pressure*	Pa	20064 (20°C)	Geometric mean
Henry coefficient	Pa m <sup>3</sup> /mol	296 (20°C)	Calculated
log Kow	g/g	1.94	Geometric mean
log Koc	dm <sup>3</sup> /kg	1.832381	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	3.00x10 <sup>-7</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.8976 (25°C)	US-EPA (1996c)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	8.64x10 <sup>-5</sup> (25°C)	US-EPA (1996c)
Kp	[cm/h]	1.66x10 <sup>-1</sup>	N Islam et al. (1996) in Fan et al. (2007)
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2B B2 3	IARC (1999c) US-EPA (2001) W EC (1993)
Systemic effects threshold			N not included in standard
TDI oral	mg/kg.d	1.0x10 <sup>-2</sup>	US-EPA (2001)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-4</sup>	W Ontario (2008)
TDI dermal	mg/kg.d	1.0x10 <sup>-2</sup>	= oral value
averaging period		child, adolescent, adult	
Systemic effects non- threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	1.5x10 <sup>-3</sup>	WHO (1996)
inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	8.6x10 <sup>-3</sup>	W OEHHA (1990); US-EPA (2001) – mean value
Dermal slop factor	(mg/kg.d) <sup>-1</sup>	1.5x10 <sup>-3</sup>	= oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	

Parameter	Unit	Value	Source
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	W

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## CHAPTER 5. SUBSTANCE DATA SHEETS CHLOROENZENES

Data on substances that do not derive from the former substance data sheets are indicated with **N**, accompanied with some explanation if appropriate. Detailed information on all new entries is given in Cornelis et al. (2013). Data on substances that differ from Flanders are indicated with **W**. Volatile pollutants (vapour pressure > 0.1Pa at 20°C) are highlighted in the document.

## 5.1. MONOCHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		108-90-7	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	112.6	
Solubility	mg/l	500 (20°C)	Verschuereen (1983)
Vapour pressure*	Pa	1173 (20°C)	Verschuereen (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	2.83	US-EPA (1994)
log Koc	dm <sup>3</sup> /kg	2.238046	US-EPA (1994)
Log Koa	g/g	calculated	<b>N</b>
BCF		calculated	
Dpe	m <sup>2</sup> /d	3.5x10 <sup>-6</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	<b>N</b>
FA	-	1	<b>N</b>
ABS dermal soil/dust	-	0.1	<b>N</b> = other chlorobenzenes
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	<b>N</b>
BTF liver	d/kg	calculated	<b>N</b>
BTF kidney	d/kg	calculated	<b>N</b>
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	<b>N</b> values not searched for
BTF feed - egg	d/kg	0	<b>N</b> values not searched for
Carcinogenicity		D	<b>W</b> US-EPA (1991)
Systemic effects threshold			
TDI oral	mg/kg.d	2.0x10 <sup>-2</sup>	<b>W</b> US-EPA (1988c)
TCL inhalation	mg/m <sup>3</sup>	2.1x10 <sup>-3</sup>	<b>W</b> Québec (2002)
TDI dermal	mg/kg.d	2.0x10 <sup>-2</sup>	<b>W</b> = oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	<b>W</b>

Parameter	Unit	Value	Source
Limit value in drinking water	mg/kg fw	-	
Limit value in plants			
Limit value in meat	mg/kg fw	-	
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day		
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 5.2. 1,2-DICHLOROBENZENE

At risk assessment, the risks of 1,2-dichlorobenzene and 1,3-dichlorobenzene must be combined. The sum of the risk indices (RI values) of both chemicals should not exceed 1.

Parameter	Unit	Value	Source
CAS nr.		95-50-1	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	147	
Solubility	mg/l	140 (20°C)	Verschuieren (1983) Kühne et al. (1995)
Vapour pressure*	Pa	200 (20°C)	Verschuieren (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	-	
log Kow	g/g	3.1	Verschuieren (1983) Kile et al. (1995)
log Koc	dm <sup>3</sup> /kg	calculated	
Log Koa	g/g	calculated	<b>N</b>
BCF		calculated	
Dpe	m <sup>2</sup> /d	2.00x10 <sup>-6</sup>	van den Berg (1994), value 1,4-dichlorobenzene
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	<b>N</b>
FA	-	1	<b>N</b>
ABS dermal soil/dust	-	0.1	<b>N</b> US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	<b>N</b>
BTF liver	d/kg	calculated	<b>N</b>
BTF kidney	d/kg	calculated	<b>N</b>
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	<b>N</b> values not searched for
BTF feed - egg	d/kg	0	<b>N</b> values not searched for
Carcinogenicity		D	<b>W</b> US-EPA (1991)
Systemic effects threshold			
TDI oral	mg/kg.d	9.0x10 <sup>-2</sup>	<b>W</b> US-EPA (1989)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-2</sup>	<b>W</b> Derived from Québec (2002) and HBEL (1995)
TDI dermal	mg/kg.d	9.0x10 <sup>-2</sup>	<b>W</b> = oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	<b>W</b>
Limit value in drinking water	mg/m <sup>3</sup>	-	<b>W</b>
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	

Parameter	Unit	Value	Source
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 5.3. 1,3-DICHLOROBENZENE

At risk assessment, the risks of 1,2-dichlorobenzene and 1,3-dichlorobenzene must be combined. The sum of the risk indices (RI values) of both chemicals should not exceed 1.

Parameter	Unit	Value	Source
CAS nr.		541-73-1	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	147	
Solubility	mg/l	130 (25°C)	Verschuieren (1983) Kühne et al. (1995)
Vapour pressure*	Pa	200 (25°C)	Verschuieren (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	-	
log Kow	g/g	3.38	Verschuieren (1983)
log Koc	dm <sup>3</sup> /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	2.00x10 <sup>-6</sup>	van den Berg (1994), value 1,4-dichlorobenzene
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	N
ABS dermal soil/dust	-	0.10	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		D	W US-EPA (1990a)
Systemic effects threshold			
TDI oral	mg/kg.d	4.29x10 <sup>-1</sup>	WHO (1993)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-2</sup>	W Derived from QC (2002) and HBEL (1995)
TDI dermal	mg/kg.d	4.29x10 <sup>-1</sup>	= oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	

Parameter	Unit	Value	Source
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day		
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)



## 5.4. 1,4-DICHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		106-46-7	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	147	
Solubility	mg/l	$4.90 \times 10^{-1}$ (22°C)	Verschuieren (1983)
Vapour pressure*	Pa	80 (20°C)	Verschuieren (1983)
Henry coefficient	Pa m <sup>3</sup> /mol	-	
log Kow	g/g	3.46	Verschuieren (1983) Mackay (1982)
log Koc	dm <sup>3</sup> /kg	2.689309	US-EPA (1994) Kile et al. (1995)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$2.00 \times 10^{-6}$	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.10	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2B 3	W IARC (1999b) W EC (2004)
Systemic effects threshold			
TDI oral	mg/kg.d	$7.0 \times 10^{-2}$	W ATSDR (2006a)
TCL inhalation	mg/m <sup>3</sup>	$6.1 \times 10^{-2}$	W ATSDR (2006a)
TDI dermal	mg/kg.d	$7.0 \times 10^{-2}$	W = oral value
averaging period		child, adolescent, adult	
Systemic effects non- threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	$4.0 \times 10^{-2}$	W OEHHA (1999b)
inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	$1.1 \times 10^{-2}$	W OEHHA (1999b)
Dermal slop factor	(mg/kg.d) <sup>-1</sup>	$4.0 \times 10^{-2}$	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	

Parameter	Unit	Value	Source
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 5.5. 1,2,4-TRICHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		120-82-1	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	181.5	
Solubility	mg/l	19 bij 22°C	Verschueren (1983)
Vapour pressure*	Pa	18.7 (20°C)	van den Berg (1994)
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	4.03	US-EPA (1994)
log Koc	dm <sup>3</sup> /kg	3.193403	US-EPA (1994)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	1.00x10 <sup>-6</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.10	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		not classified	W
Systemic effects threshold			
TDI oral	mg/kg.d	1.6x10 <sup>-3</sup>	W Health Canada (2004)
TCL inhalation	mg/m <sup>3</sup>	4.0x10 <sup>-3</sup>	W Québec (2002)
TDI dermal	mg/kg.d	1.6x10 <sup>-3</sup>	W = oral TDI
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	

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Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 5.6. 1,2,3,4-TETRACHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		634-66-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	215.9	
Solubility	mg/l	3.50 (22°C)	Verschueren (1983)
Vapour pressure*	Pa	0.534 (20°C)	van den Berg (1994)
Henry coefficient	Pa m <sup>3</sup> /mol	-	
log Kow	g/g	4.6	Chiou (1985)
log Koc	dm <sup>3</sup> /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	1.00x10 <sup>-6</sup>	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.10	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		not classified	W
Systemic effects threshold			
TDI oral	mg/kg.d	3.4x10 <sup>-3</sup>	W Health Canada (2004)
TCL inhalation	mg/m <sup>3</sup>	4.0x10 <sup>-4</sup>	W Québec (2002)
TDI dermal	mg/kg.d	3.4x10 <sup>-3</sup>	W = oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	

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Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 5.7. PENTACHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		608-93-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	250.3	
Solubility	mg/l	$5.60 \times 10^{-1}$ (25°C)	Kühne et al. (1995)
Vapour pressure*	Pa	0.133 (20°C)	van den Berg (1994)
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	5.19	Mackay (1982)
log Koc	dm <sup>3</sup> /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$1.00 \times 10^{-6}$	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.10	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		D	W US-EPA (1995)
Systemic effects threshold			
TDI oral	mg/kg.d	$8 \times 10^{-4}$	US-EPA (1988d)
TCL inhalation	mg/m <sup>3</sup>	$2.8 \times 10^{-3}$	W calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	$8 \times 10^{-4}$	= oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	

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Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)



## 5.8. HEXACHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		118-74-1	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	284.79	
Solubility	mg/l	$1.13 \times 10^{-2}$	Geometric mean
Vapour pressure	Pa	0.00187	Geometric mean
Henry coefficient	Pa m <sup>3</sup> /mol	47.5	calculated
log Kow	g/g	5.69	Geometric mean
log Koc	dm <sup>3</sup> /kg	4.692732	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$3.00 \times 10^{-7}$	van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.468	US-EPA (1996c)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	$5.04 \times 10^{-5}$	US-EPA (1996c)
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	$1.00 \times 10^{-1}$	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2B B2 2	IARC (2001) US-EPA (1996b) EC (1996)
Systemic effects threshold			
TDI oral	mg/kg.d	$7.0 \times 10^{-5}$	W ATSDR (2015)
TCL inhalation <sup>a)</sup>	mg/m <sup>3</sup>	$2.45 \times 10^{-4}$	W calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	$7.0 \times 10^{-5}$	W = oral value
averaging period	child, adolescent, adult		
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	1.8	W OEHA (1999c)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	$5.1 \times 10^{-1}$	W OEHA (1999c)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	1.8	W = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	W
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	

Parameter	Unit	Value	Source
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	




- a) The original substance data sheets express the reference value for inhalation in units of mg/kg.d. S-Risk uses a reference value in units of mg/m<sup>3</sup>. Conversion can be done by multiplying the value in mg/kg.d with a body weight of 70 kg and an inhalation rate of 20 m<sup>3</sup>/d.

## CHAPTER 6. SUBSTANCE DATA SHEETS CHLOROPHENOLS

Data on substances that do not derive from the former substance data sheets are indicated with **N**, accompanied with some explanation if appropriate. Detailed information on all new entries is given in Cornelis et al. (2013). Data on substances that differ from Flanders are indicated with **W**. Volatile pollutants (vapour pressure > 0.1Pa at 20°C) are highlighted in the document.

## 6.1. 2-CHLOROPHENOL

Parameter	Unit	Value	Source
CAS nr.		95-57-8	
Type		organic	
Dissociating		yes	
Acid dissociation		yes	
pKa		8.47	
Molecular weight	g/mol	128.56	Mackay et al (1995)
Solubility	mg/l	1.86x10 <sup>4</sup> (25°C)	average
Vapour pressure*	Pa	294 (25°C)	average
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	2.13	average
log Koc	dm <sup>3</sup> /kg	not used	dissociating
Log Koa	g/g	calculated	<b>N</b>
BCF		calculated	
Dpe	m <sup>2</sup> /d	5.00x10 <sup>-9</sup>	Lijzen et al. (2001)
Dpvc	m <sup>2</sup> /d	5.00x10 <sup>-12</sup>	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.432	RAIS-online
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	8.18x10 <sup>-5</sup>	RAIS-online
Kp	[cm/h]	calculated	<b>N</b>
FA	-	1	<b>N</b>
ABS dermal soil/dust	-	0.1	<b>N</b> RAIS-online
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	<b>N</b>
BTF liver	d/kg	calculated	<b>N</b>
BTF kidney	d/kg	calculated	<b>N</b>
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	<b>N</b> rapid screening did not provide values
BTF feed - egg	d/kg	0	<b>N</b> rapid screening did not provide values
Carcinogenicity		2B	IARC (1999a) (polychlorophenoles)
Systemic effects threshold			
TDI oral	mg/kg.d	5x10 <sup>-3</sup>	US-EPA-IRIS (1993)

Parameter	Unit	Value	Source
TCL inhalation	mg/m <sup>3</sup>	7.0x10 <sup>-3</sup>	 Derived from US-EPA (1988a)
TDI dermal	mg/kg.d	5x10 <sup>-3</sup>	= oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 6.2. 2,4-DICHLOROPHENOL

Parameter	Unit	Value	Source
CAS nr.		102-83-2	
Type		Organic	
Dissociating		yes	
Acid dissociation		yes	
pKa		7.9	
Molecular weight	g/mol	163.01	Mackay et al (1995)
Solubility	mg/l	4.87x10 <sup>3</sup> (25°C)	average
Vapour pressure*	Pa	25.5 (25°C)	average
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	3.08	average
log Koc	dm <sup>3</sup> /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m <sup>2</sup> /d	1.00x10 <sup>-7</sup>	Lijzen et al. (2001)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.3	RAIS-online
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	7.58x10 <sup>-5</sup>	RAIS-online
Kp	[cm/h]	NaN	
FA	-	1	
ABS dermal soil/dust	-	0.1	RAIS-online
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	
BTF kidney	d/kg	calculated	
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	rapid screening does not provide values
BTF feed - egg	d/kg	0	rapid screening does not provide values
Carcinogenicity		2B	IARC (1999a) (polychlorophenols)
Systemic effects threshold			
TDI oral	mg/kg.d	3.0x10 <sup>-3</sup>	US-EPA-IRIS (1988b)
TCL inhalation	mg/m <sup>3</sup>	3.0x10 <sup>-3</sup>	Québec (2002)
TDI dermal	mg/kg.d	3.0x10 <sup>-3</sup>	= oral TDI
averaging period		Child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	

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Parameter	Unit	Value	Source
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 6.3. 2,4,5-TRICHLOROPHENOL

Parameter	Unit	Value	Source
CAS nr.		95-95-4	
Type		organic	
Dissociating		yes	
Acid dissociation		yes	
pKa		6.98	
Molecular weight	g/mol	197.45	Mackay et al (1995)
Solubility	mg/l	1.08x10 <sup>3</sup> (25°C)	average
Vapour pressure*	Pa	4.77 (25°C)	average
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	3.72	average
log Koc	dm <sup>3</sup> /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m <sup>2</sup> /d	5.00x10 <sup>-7</sup>	Lijzen et al. (2001)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.252	RAIS-online
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	6.07E-05	RAIS-online
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0.1	RAIS-online
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	
BTF kidney	d/kg	calculated	
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	rapid screening did not provide values
BTF feed - egg	d/kg	0	rapid screening did not provide values
Carcinogenicity		2B	IARC (1999a) (polychlorophenols)
Systemic effects threshold			
TDI oral	mg/kg.d	1.0x10 <sup>-1</sup>	US-EPA (1991)
TCL inhalation	mg/m <sup>3</sup>	1.0x10 <sup>-1</sup>	Québec (2002)
TDI dermal	mg/kg.d	1.0x10 <sup>-1</sup>	= oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	

Parameter	Unit	Value	Source
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)



## 6.4. 2,4,6-TRICHLOROPHENOL

Parameter	Unit	Value	Source
CAS nr.		88-06-2	
Type		organic	
Dissociating		yes	
Acid dissociation		yes	
pKa		6.12	
Molecular weight	g/mol	197.45 (25°C)	Mackay et al (1995)
Solubility	mg/l	5.97x10 <sup>2</sup> (25°C)	average
Vapour pressure*	Pa	2.66	average
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	3.54	average
log Koc	dm <sup>3</sup> /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m <sup>2</sup> /d	5.00x10 <sup>-7</sup>	Lijzen et al. (2001)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.2736	RAIS-online
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	0.000054	RAIS-online
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0.1	RAIS-online
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	
BTF kidney	d/kg	calculated	
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	rapid screening did not provide values
BTF feed - egg	d/kg	0	rapid screening did not provide values
Carcinogenicity		2B	IARC (1999a) (polychlorophenols)
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	7.0x10 <sup>-2</sup>	OEHTA (2009)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	6.0x10 <sup>-3</sup>	US-EPA (1990b); OEHTA (1999); Québec (2002) – mean value
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	7.0x10 <sup>-2</sup>	= oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	

Parameter	Unit	Value	Source
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 6.5. 2,3,4,6-TETRACHLOROPHENOL

Parameter	Unit	Value	Source
CAS nr.		58-90-2	
Type		organic	
Dissociating		yes	
Acid dissociation		yes	
pKa		5.4	
Molecular weight	g/mol	231.89 (25°C)	Mackay et al (1995)
Solubility	mg/l	1.54x10 <sup>2</sup> (25°C)	average
Vapour pressure*	Pa	0.64	average
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	4.32	average
log Koc	dm <sup>3</sup> /kg	not used	dissociating
Log Koa	g/g	calculated	<input type="checkbox"/>
BCF		calculated	
Dpe	m <sup>2</sup> /d	1.00x10 <sup>-6</sup>	Lijzen et al. (2001)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.18744	RAIS-online
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	6.14x10 <sup>-5</sup>	RAIS-online
Kp	[cm/h]	calculated	<input type="checkbox"/>
FA	-	1	<input type="checkbox"/>
ABS dermal soil/dust	-	0.1	<input type="checkbox"/> RAIS-online
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	<input type="checkbox"/>
BTF liver	d/kg	calculated	<input type="checkbox"/>
BTF kidney	d/kg	calculated	<input type="checkbox"/>
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	<input type="checkbox"/> rapid screening did not provide values
BTF feed - egg	d/kg	0	<input type="checkbox"/> rapid screening did not provide values
Carcinogenicity		2B	IARC (1999a) (polychlorophenols)
Systemic effects threshold			
TDI oral	mg/kg.d	1.0x10 <sup>-2</sup>	<input checked="" type="checkbox"/> Health Canada (2004)
TCL inhalation	mg/m <sup>3</sup>	0.35	<input checked="" type="checkbox"/> calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	1.0x10 <sup>-2</sup>	<input checked="" type="checkbox"/> = oral value
averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	<input checked="" type="checkbox"/>
Limit value in drinking water	mg/m <sup>3</sup>	-	<input checked="" type="checkbox"/>
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	

Parameter	Unit	Value	Source
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	
Dietary background children	mg/kg.day	0	
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

\* Volatile pollutant (vapour pressure > 0.1Pa at 20°C)

## 6.6. PENTACHLOROPHENOL

Parameter	Unit	Value	Source
CAS nr.		87-86-5	
Type		organic	
Dissociating		yes	
Acid dissociation		yes	
pKa		4.9	
Molecular weight	g/mol	266.34	Mackay et al (1995)
Solubility	mg/l	17.2 (25°C)	average
Vapour pressure	Pa	0.09 (25°C)	average
Henry coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	4.81	average
log Koc	dm <sup>3</sup> /kg	not used	dissociating
Log Koa	g/g	calculated	<input type="checkbox"/>
BCF		calculated	
Dpe	m <sup>2</sup> /d	2.24x10 <sup>-6</sup>	Lijzen et al. (2001)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.48	RAIS-online
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	5.28x10 <sup>-5</sup>	RAIS-online
Kp	[cm/h]	calculated	<input type="checkbox"/>
FA	-	0.9	<input type="checkbox"/> US-EPA, 2004
ABS dermal soil/dust	-	2.50x10 <sup>-1</sup>	<input type="checkbox"/> RAIS-online
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	<input type="checkbox"/>
BTF liver	d/kg	calculated	<input type="checkbox"/>
BTF kidney	d/kg	calculated	<input type="checkbox"/>
BTF milk	d/kg	calculated	
BTF soil - egg	d/kg	0	<input type="checkbox"/> rapid screening did not provide values
BTF feed - egg	d/kg	0	<input type="checkbox"/> rapid screening did not provide values
Carcinogenicity		2B Likely to be carcinogenic to humans	IARC (1999a) (polychlorophenols) <input type="checkbox"/> US-EPA (2010a)
Systemic effects threshold			
TDI oral	mg/kg.d	1.0x10 <sup>-3</sup>	<input type="checkbox"/> ATSDR (2001)
TCL inhalation <sup>a)</sup>	mg/m <sup>3</sup>	3.5x10 <sup>-3</sup>	<input type="checkbox"/> calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	1.0x10 <sup>-3</sup>	<input type="checkbox"/> = oral value
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	4.0x10 <sup>-1</sup>	<input type="checkbox"/> US-EPA (2010a)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	1.1x10 <sup>-1</sup>	Derived from US-EPA (2010a))
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	4.0x10 <sup>-1</sup>	<input type="checkbox"/> = oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	<input type="checkbox"/>
Limit value in plants	mg/kg fw	-	<input type="checkbox"/>
Limit value in meat			<input type="checkbox"/>

Parameter	Unit	Value	Source
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	
Background root crops	mg/kg fw	0	
Background bulbous plants (onion ...)	mg/kg fw	0	
Background fruit vegetables	mg/kg fw	0	
Background cabbage	mg/kg fw	0	
Background leafy vegetables	mg/kg fw	0	
Background legume	mg/kg fw	0	
Background beef	mg/kg fw	0	
Background offal	mg/kg fw	0	
Background milk	mg/kg fw	0	
Background butter	mg/kg fw	0	
Background eggs	mg/kg fw	0	
Background outdoor air	mg/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

- a) The original substance data sheets express the reference value for inhalation in units of mg/kg.d. S-Risk uses a reference value in units of mg/m<sup>3</sup>. Conversion can be done by multiplying the value in mg/kg.d with a body weight of 70 kg and an inhalation rate of 20 m<sup>3</sup>/d.

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