

Final report

S-Risk 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
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
VMM	Vlaamse MilieuMaatschappij (Flanders Environment Agency)

LIST OF MODIFICATIONS

28/09/2016	The CAS number for trichloroethylene was corrected
12/01/2017	The CAS number of monochlorobenzene was corrected
07/02/2017	Typos corrected
15/05/2019	Update of substance data dichloromethane, tetrachloromethane, tetrachloroethylene, trichloroethylene and 1,1,1-trichloroethane and update of 'introduction'

INTRODUCTION

The substance data sheets summarise the data as available in S-Risk 1.0. The substance data sheets are a copy of those used for the calculation of the proposed soil clean-up values in Flanders. 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/m³ 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, dichloromethane, tetrachloromethane, tetrachloroethylene, trichloroethylene and 1,1,1-trichloroethane 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 ratio's 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 1,1,2-trichloroethane, 1,1-dichloroethane, cis-1,2-dichloroethene, trans-1,2-dichloroethene; Van Holderbeke, Geerts, Bierkens, and Cornelis (2019) for 1,1,1-trichloroethane, dichloromethane, tetrachloroethylene, tetrachloromethane, trichloroethylene; 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 for benzo(a)pyrene and dibenz(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 is always available in the report discussing the calculation of clean-up values with S-Risk (Cornelis, Bierkens, & Standaert, 2013). Newly added or modified information compared to the original data sheets is clearly indicated in the S-Risk substance data sheets.

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 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).








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


Chemical name	Report
Dichloromethane	Van Holderbeke, Geerts, Bierkens, and Cornelis (2019)
Tetrachloromethane	Van Holderbeke, Geerts, Bierkens, and Cornelis (2019)
Tetrachloroethylene	Van Holderbeke, Geerts, Bierkens, and Cornelis (2019)
Trichloroethylene	Van Holderbeke, Geerts, Bierkens, and Cornelis (2019)
1,1,1-trichloroethane	Van Holderbeke, Geerts, Bierkens, and Cornelis (2019)
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	1.99x10 ⁴ (25°C)	Kühne et al. (1995)
Vapour pressure	Pa	57662 (25°C)	Average of experimental data and calculated with Antoine equation
Henry coefficient	Pa m ³ /mol	134 (10°C)	Regression from Warneck (2007)
log Kow	g/g	1.3 (K _{ow} = 20)	Average of experimental and QSAR data
log Koc	dm ³ /kg	calculated	Calculated in S-Risk (hydrophobic chemical)
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	5 x 10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0	 negligible, volatile chemical
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	0.33	Leeman et al. (2007)
BTF feed - egg	d/kg	0.33	Leeman et al. (2007)
Carcinogenicity		2A	IARC (2014)
Systemic effects threshold			
TDI oral	mg/kg.d	6 x 10 ⁻³	WHO (2003), US-EPA (2011)
TCL inhalation	mg/m ³	6 x 10 ⁻¹	US-EPA (2011)
TDI dermal	mg/kg.d	6 x 10 ⁻³	same as oral TDI
averaging period		child, adolescent, adult	
Carcinogenicity (unit risk)			
Oral slope factor	(mg/kg.d) ⁻¹	2 x 10 ⁻³ (adult) 6 x 10 ⁻³ (3 - < 15 yr) 2 x 10 ⁻² (1 - < 3 yr)	US-EPA (2011) ^{a)}
Inhalation unit risk	(mg/m ³) ⁻¹	1 x 10 ⁻⁵ (volw) 3 x 10 ⁻⁵ (3 - < 15 yr) 1 x 10 ⁻⁴ (1 - < 3 yr)	US-EPA (2011) ^{a)}

Parameter	Unit	Value	Source
Dermal slope factor	(mg/kg.d) ⁻¹	2 × 10 ⁻³ (adult) 6 × 10 ⁻³ (3 - < 15 yr) 2 × 10 ⁻² (1 - < 3 yr)	= Oral slope factor
averaging period		lifelong	
Local effects threshold			
inhalation	(mg/m ³)	4,5 × 10 ⁻¹	WHO (2000)
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	0.45	WHO (2000) ^b , toxicological reference value
Limit value in drinking water	mg/m ³	20	WHO (1993)
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 ³	0	no values
Background indoor air	mg/m ³	0	 no values
Background drinking water	mg/m ³	0.1	VROM (2010)

- a) Because the studies do not include early life stages, US-EPA proposes to multiply the unit risk and the slope factor by age dependent factors (factor 10 for <2 years, factor 3 for 2-<16 years and factor 1 for ≥ 16 years) to take into account the possible increased sensitivity during childhood.
- b) The lifelong slope factor for inhalation is 1.7·10⁻⁵ (mg / m³)⁻¹ (US-EPA, 2011). Converted to an extra lifelong cancer risk of 1·10⁻⁵, this results in a concentration of 0.60 mg / m³. The value based on the formation of COHb (0.45 mg / m³) is lower and is therefore selected.

4.2. TETRACHLOROMETHANE

Parameter	Unit	Value	Source
CAS nr.		56-23-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	154	
Solubility	mg/l	775 (25°C)	Average of experimental data
Vapour pressure	Pa	14991 (25°C)	Average of experimental data and calculated with Antoine equation
Henry coefficient	Pa m ³ /mol	1310 (10°C)	Regression, Warneck (2007)
log Kow	g/g	2.66 (K _{ow} = 457)	Average of experimental data
log Koc	dm ³ /kg	1.79 (K _{oc} = 62)	Average of experimental data for soils with OC ≥ 0,3 %
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	8 x 10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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	1.06	Leeman et al. (2007)
BTF feed - egg	d/kg	1.06	Leeman et al. (2007)
Carcinogenicity		2B	IARC (1999b)
Systemic effects threshold			
TDI oral	mg/kg.d	4 × 10 ⁻³	IRIS US-EPA (2010)
TCL inhalation	mg/m ³	1 × 10 ⁻¹	IRIS US-EPA (2010))
TDI dermal	mg/kg.d	4 × 10 ⁻³	oral TDI
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	0.1	IRIS US-EPA (2010) Toxicological reference value
Limit value in drinking water	mg/m ³	12	IRIS US-EPA (2010) Toxicological reference value
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	No recent data
Dietary background children	mg/kg.day	0	No recent data
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 ³	1 × 10 ⁻³	Health Canada (2010)
Background indoor air	mg/m ³	1 × 10 ⁻³	= outdoor air
Background drinking water	mg/m ³	0	 no values

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	3.12×10^2 (25°C)	Average of experimental data
Vapour pressure	Pa	2609 (25 °C)	Average of experimental data and calculated with Antoine equation
Henry coefficient	Pa m ³ /mol	822 (10°C)	Regression, Warneck (2007)
log Kow	g/g	2.75 (K _{ow} = 562)	Average of experimental data
log Koc	dm ³ /kg	2.10 (K _{oc} = 126)	Average of experimental data
Log Koa	g/g	calculated	☒
BCF		calculated	
Dpe	m ² /d	7.7×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	1.41×10^{-1}	☒ Frasch en Barbero (2009)
FA	-	1	☒
ABS dermal soil/dust	-	3.00×10^{-2}	☒ US-EPA (1995b, 2003)
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	1.06	Leeman, Van den Berg, and Houben (2007)
BTF feed - egg	d/kg	1.06	Leeman, Van den Berg, and Houben (2007)
Carcinogenicity		2A	IARC (2014)
Systemic effects threshold			
TDI oral	mg/kg.d	5×10^{-2}	WHO (2006)
TCL inhalation ^{a)}	mg/m ³	0.25	WHO (2000)
TDI dermal	mg/kg.d	5×10^{-2}	= oral TDI
averaging period		child, adolescent, adult	
Carcinogenicity (unit risk)			
Oral slope factor	(mg/kg.d) ⁻¹	2.1×10^{-3}	US-EPA (2012)
Inhalation unit risk	(mg/m ³) ⁻¹	2.6×10^{-4}	US-EPA (2012)
Dermal slope factor	(mg/kg.d) ⁻¹	2.1×10^{-3}	= oral slope factor
averaging period		lifelong	

Parameter	Unit	Value	Source
Limit value in air	mg/m ³	3.8 × 10 ⁻² outdoor air	US-EPA (2012) Derived from unit risk BS (2004), richtwaarde binnenmilieu
		1 × 10 ⁻¹ indoor air	
Limit value in drinking water	mg/m ³	10	(BS, 2003), sum of tri- en tetrachloroethylene
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	1.89 × 10 ⁻³	Medeiros Vinci, Jacxsens, De Meulenaere, Deconink, Matsiko, Lachat, et al. (2015) and consumption data EFSA
Dietary background children	mg/kg.day	1-<3: 6.23 × 10 ⁻³ 3-<6: 5.18 × 10 ⁻³ 6-<10: 5.18 × 10 ⁻³ 10-<15: 2.20 × 10 ⁻³ 15-<21: 2.04 × 10 ⁻³ >21: 1.89 × 10 ⁻³	Medeiros Vinci, et al. (2015) (average concentrations) and consumption data EFSA
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 ³	1.00 × 10 ⁻⁴	VMM (2014)
Background indoor air	mg/m ³	1.00 × 10 ⁻⁴	☒ = outdoor air
Background drinking water	mg/m ³	0	☒ no values



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	1372 (25°C)	Average of experimental data
Vapour pressure	Pa	9635 (25°C)	Average of experimental data and calculated with Antoine equation
Henry coefficient	Pa m ³ /mol	439 (10°C)	Average of experimental data
log Kow	g/g	2.52 (K _{ow} = 331)	Average of experimental data
log Koc	dm ³ /kg	1.994 (K _{oc} = 98)	Average of experimental data
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	1.60x10 ⁻⁶	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	1.20 x 10 ⁻¹	 Nakai et al. (1999)
FA	-	1	
ABS dermal soil/dust	-	5.90 x 10 ⁻³	 derived from Poet et al. (2000) en Spalt et al. (2009)
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	1.06	Derived from Leeman et al. (2007)
BTF feed - egg	d/kg	1.06	Derived from Leeman et al. (2007)
Carcinogenicity		1	IARC (2014)
Systemic effects threshold			
TDI oral	mg/kg.d	1.46 x 10 ⁻³	WHO (2005)
TCL inhalation	mg/m ³	6 x 10 ⁻¹	(OEHHA 2008)
TDI dermal	mg/kg.d	1.46 x 10 ⁻³	= oral TDI
averaging period		child, adolescent, adult	
Carcinogenicity (unit risk)			
Oral slope factor	(mg/kg.d) ⁻¹	7.8 x 10 ⁻⁴	WHO (2005)
Inhalation unit risk	(mg/m ³) ⁻¹	4.3 x 10 ⁻⁴	WHO (2000)
Dermal slope factor	(mg/kg.d) ⁻¹	7.8 x 10 ⁻⁴	= oral slope factor
averaging period		lifelong	

Parameter	Unit	Value	Source
Limit value in air	mg/m ³	2.3 × 10 ⁻² outdoor air	Toxicological value (derived from unit risk WHO (2000) 1:10 ⁶)
		2 × 10 ⁻¹ indoor air	BS (2004), richtwaarde binnenmilieu
Limit value in drinking water	mg/m ³	10	BS (2003), sum of tri- en tetrachloroethylene
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	3.05 × 10 ⁻⁵	Medeiros Vinci, et al. (2015) and consumptiondata EFSA
Dietary background children	mg/kg.day	1-<3: 3.23 × 10 ⁻⁴ 3-<6: 2.51 × 10 ⁻⁴ 6-<10: 2.51 × 10 ⁻⁴ 10-<15: 4.08 × 10 ⁻⁵ 15-<21: 3.57 × 10 ⁻⁵ >21: 3.05 × 10 ⁻⁵	Medeiros Vinci, et al. (2015) and consumptiondata EFSA
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 ³	2.00 × 10 ⁻⁴	▮ data for the Netherlands (2006-2008)
Background indoor air	mg/m ³	2.00 × 10 ⁻⁴	▮ = outdoor air
Background drinking water	mg/m ³	0	No values



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	1430 (25°C)	average of experimental data
Vapour pressure	Pa	16540 (25°C)	Average of experimental data and calculated with Antoine equation
Henry coefficient	Pa m ³ /mol	830 (10°C)	average of experimental data
log K _{ow}	g/g	2.42 (K _{ow} = 263)	average of experimental data
log K _{oc}	dm ³ /kg	2.01 (K _{oc} = 102)	average of experimental data
Log K _{oa}	g/g	calculated	N
BCF		calculated	
D _{pe}	m ² /d	2.00 x 10 ⁻⁶	Kreule et al. (1995)
D _{pvc}	m ² /d	2.00 x 10 ⁻⁹	
Diffusion coefficient air (D _a)	m ² /d	calculated	
Diffusion coefficient water (D _w)	m ² /d	calculated	
K _p	[cm/h]	1.67 x 10 ⁻¹	N Fan et al. (2007)
FA	-	1	Geerts, Bierkens, Cornelis, and Gemoets (2011)
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	1.06	Derived from Leeman et al. (2007)
BTF feed - egg	d/kg	1.06	Derived from Leeman et al. (2007)
Carcinogenicity		3	IARC (1987)
Systemic effects threshold			
TDI oral	mg/kg.d	6 x 10 ⁻¹	WHO (2003)
TCL inhalation	mg/m ³	1	OEHHA (2006)
TDI dermal	mg/kg.d	6 x 10 ⁻¹	= oral TDI
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1	TCL inhalation
Limit value in drinking water	mg/m ³	2000	WHO (2011)
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	7.82×10^{-4}	Medeiros Vinci, et al. (2015) and consumption data EFSA
Dietary background children	mg/kg.day	1-<3: 3.47×10^{-3} 3-<6: 2.74×10^{-3} 6-<10: 2.74×10^{-3} 10-<15: 8.76×10^{-4} 15-<21: 8.29×10^{-4} >21: 7.82×10^{-4}	Medeiros Vinci, et al. (2015) and consumption data EFSA
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 ³	$1.00 \cdot 10^{-4}$	VMM (2014)
Background indoor air	mg/m ³	$1.00 \cdot 10^{-4}$	 = outdoor air
Background drinking water	mg/m ³	0	 no values

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 ³ (20°C)	average of 4 data points
Vapour pressure	Pa	2533 (20°C)	average of 6 measurements
Henry coefficient	Pa m ³ /mol	80 (10°C)	Average of 4 measurements
log Kow	g/g	2.1	average of 6 data points
log Koc	dm ³ /kg	1.8	average of 12 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.00x10 ⁻⁶	= value 1,1,1-trichloroethane
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	8.40x10 ⁻²	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 (1991)
Systemic effects threshold			
TDI oral	mg/kg.d	4x10 ⁻³	US-EPA (1995a)
TCL inhalation ^{a)}	mg/m ³	3.9x10 ⁻²	Hassauer et al. (1993)
TDI dermal	mg/kg.d	4x10 ⁻³	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	3.90x10 ⁻²	Hassauer et al. (1993)
Limit value in drinking water	mg/m ³	12	calculated from oral TDI
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	

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 ³	4.90x10 ⁻⁴	Van de Plassche et al. (1993)
Background indoor air	mg/m ³	4.90x10 ⁻⁴	 = outdoor air
Background drinking water	mg/m ³	0	 no values

- 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/m³. 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 m³/d.

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	5.40x10 ³ (20°C)	average of 5 data points
Vapour pressure	Pa	25771 (20°C)	regression on 13 data
Henry coefficient	Pa m ³ /mol	249 (10°C)	regression on 15 data
log Kow	g/g	1.79	average of 7 data points
log Koc	dm ³ /kg	1.55	average of 6 data points
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	3.00x10 ⁻⁷	Kreule et al (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	2.59x10 ⁻¹	= value 1,2-dichloroethane
FA	-	1	
ABS dermal soil/dust	-	0	negligible, volatile chemical
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	values not searched for
BTF feed - egg	d/kg	0	values not searched for
Carcinogenicity		3	IARC (?), cannot be traced back
Systemic effects threshold			
TDI oral	mg/kg.d	8x10 ⁻²	Kreule et al. (1995)
TCL inhalation ^{a)}	mg/m ³	3.7x10 ⁻¹	Janssen et al. (1995)
TDI dermal	mg/kg.d	8x10 ⁻²	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	3.70x10 ⁻¹	Janssen et al. (1995)
Limit value in drinking water	mg/m ³	240	from oral TDI
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	5.00x10 ⁻⁵	?, cannot be traced back
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	Cornelis et al. (2013)
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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

4.8. 1,2-DICHLOROETHANE

! The toxicological data that have been used in the calculation of the clean-up values and the data that were used in Vlier-Humaan differ significantly with regard to 1,2-dichloroethane. The data used in Vlier-Humaan and listed in the original data sheet result in higher risks. The footnote to the below substance data sheet gives further clarification. At present, it is clear that 1,2-dichloroethane should be considered a carcinogen by all routes of exposure. An evaluation of the most recent toxicological data is required.

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 ³ (20°C)	Geometric mean
Vapour pressure	Pa	8528 (20°C)	Geometric mean
Henry coefficient	Pa m ³ /mol	98.23 (20°C)	calculated
log Kow	g/g	1.52	Geometric mean
log Koc	dm ³ /kg	1.418798	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	3.00x10 ⁻⁷	Van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.888	US-EPA, (1996c)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	US-EPA, (1996c)
Kp	[cm/h]	2.59x10 ⁻¹	N Frasc en 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 (1979) US-EPA (1991a)
Local effects threshold ^{a)}			N different from Vlier-Humaan
TCL inhalation	mg/m ³	7x10 ⁻¹	WHO (2000)
Systemic effects no threshold ^{a,b)}			N cfr. clean-up values, different from Vlier-Humaan
Oral slope factor	(mg/kg.d) ⁻¹	1x10 ⁻²	WHO (1993)
Inhalation unit risk	(mg/m ³) ⁻¹	1x10 ⁻⁸	dummy value (considered non-carcinogenic by inhalation)
Dermal slope factor	(mg/kg.d) ⁻¹	1x10 ⁻²	= oral value
Limit in air ^{a)}	mg/m ³	7x10 ⁻¹	N WHO (2000)
Limit value in drinking water	mg/m ³	30	WHO (1996)
Limit value in plants	mg/kg fw	0.01 (alle producten)	Detection limit, EC (2005)
Limit value in meat			

Parameter	Unit	Value	Source
Beef	mg/kg fw	0.1	Detection limit, EC (2005)
Mutton	mg/kg fw	0.1	Detection limit, EC (2005)
Liver	mg/kg fw	0.1	Detection limit, EC (2005)
Kidney	mg/kg fw	0.1	Detection limit, EC (2005)
Milk	mg/kg fw	0.1	Detection limit, EC (2005)
Butter	mg/kg fw	0.1	Detection limit, EC (2005)
Egg	mg/kg fw	0.1	Detection limit, EC (2005)
Dietary background adults	mg/kg day	0	WHO (2000)
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 ³	1.20x10 ⁻³	VMM (1999, 2000)
Background indoor air	mg/m ³	1.20x10 ⁻³	 = outdoor air
Background drinking water	mg/m ³	5.00x10 ⁻²	 VMM (2006)

- a) When calculating the clean-up values, a toxicological reference value for oral carcinogenicity and inhalation non-carcinogenicity was used for 1,2-dichloroethane. The chemical was considered a carcinogen, which means that lifelong exposure was calculated. To fill this in the S-Risk data format, 1,2-dichloroethane is entered as a systemic carcinogen without threshold with a very low slope factor for the inhalation route (dummy value). Consequently, the oral and dermal route are accounted for in the carcinogenic effects and the inhalation route contributes only to a negligible extent. With regard to inhalation, local effects are considered as well, with the toxicological reference value from the calculation of the clean-up values. The limit in air corresponds to the value for non-carcinogenic effects.
- Vlier-Humaan and the associated data sheet (part of the current 'Basisinformatie voor risico-evaluaties' – version 2014) list the data at which 1,2-dichloroethane is considered a carcinogen by all exposure routes. If these data would be copied, this would give following S-Risk input:
- Oral systemic without threshold: 0.01 (mg/kg.d)⁻¹
 - Inhalation systemic without threshold: 2.6.10⁻² (mg/m³)⁻¹
 - Dermal systemic without threshold: 0.01 (mg/kg.d)⁻¹ (oral absorption factor: 1)
- Limiet in air : 4.10⁻⁴ mg/m³
 Limiet in drinking water: 30 mg/m³
- b) The original substance data sheet lists the reference values for carcinogenic non-threshold effects as a dose corresponding to an excess lifelong cancer risk of 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(dose at 1.10⁻⁵ (mg/kg.d)). In case of inhalation risks, the dose is first converted to a concentration by multiplying it with 70 kg (body weight) and dividing it by 20 m³/d (inhalation rate).

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 ³ /mol	226 (10°C)	regression on 8 data
log Kow	g/g	1.14	average of 4 data points
log Koc	dm ³ /kg	1.67	average of 4 data points
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	4.00x10 ⁻⁸	Kreule et al. (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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		Not evaluated D	IARC (1998)? IRIS (1998)?
Systemic effects threshold			
TDI oral	mg/kg.d	1.7x10 ⁻²	WHO (1996)
TCL inhalation ^{a)}	mg/m ³	3x10 ⁻²	Kreule et al. (1995)
TDI dermal	mg/kg.d	1.7x10 ⁻²	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	3.00x10 ⁻²	Kreule et al. (1995)
Limit value in drinking water	mg/m ³	50	WHO (1996)
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	1.50x10 ⁻⁴	Kreule et al. (1995)
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	N Cornelis et al. (2013)

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 ³	4.00x10 ⁻⁵	WHO (1996)
Background indoor air	mg/m ³	4.00x10 ⁻⁵	<input checked="" type="checkbox"/> = outdoor air
Background drinking water	mg/m ³	0	<input checked="" type="checkbox"/> no values

- 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/m³. 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 m³/d.

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 ³ /mol	449 (10°C)	regression on 11 data
log Kow	g/g	1.41	average of 3 data points
log Koc	dm ³ /kg	1.68	average of 3 data points
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	4.00x10 ⁻⁸	Kreule et al (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0	negligible, volatile chemical
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	values not searched for
BTF feed - egg	d/kg	0	values not searched for
Carcinogenicity		Not evaluated D	IARC (1998)? IRIS (1998)?
Systemic effects threshold			
TDI oral	mg/kg.d	1.7x10 ⁻²	WHO (1996)
TCL inhalation ^{a)}	mg/m ³	8x10 ⁻²	Kreule et al. (1995)
TDI dermal	mg/kg.d	1.7x10 ⁻²	= oral value
averaging period	mg/m ³	8.00x10 ⁻²	Kreule et al. (1995)
Limit value in air	mg/m ³	50	WHO (1996)
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	1.50x10 ⁻⁴	Kreule et al. (1995)
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	Cornelis et al. (2013)
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 ³	1.03x10 ⁻²	WHO (1996)
Background indoor air	mg/m ³	1.03x10 ⁻²	 = outdoor air
Background drinking water	mg/m ³	0	 no values

- 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/m³. 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 m³/d.

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 ³ /mol	18637 (20°C)	Calculated
log Kow	g/g	1.24	Geometric mean
log Koc	dm ³ /kg	1.080987	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	3.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.912 (25°C)	US-EPA (1996c)
Diffusion coefficient water (Dw)	m ² /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	IARC (1979) US-EPA (2000)
Systemic effects threshold ^{a)}			N Supplementary to Vlier-Humaan data
TDI oral	mg/kg.d	3x10 ⁻³	US-EPA (2000)
TCL inhalation ^{b)}	mg/m ³	1x10 ⁻¹	US-EPA (2000)
TDI dermal	mg/kg.d	3x10 ⁻³	= oral value
averaging period		child, adolescent, adult	
Systemic effects no threshold ^{c)}			
Oral slope factor	(mg/kg.d) ⁻¹	6x10 ⁻²	WHO (1996)
Inhalation unit risk	(mg/m ³) ⁻¹	1x10 ⁻³	WHO (2000)
Dermal slope factor	(mg/kg.d) ⁻¹	6x10 ⁻²	= oral value
Limit value in air	mg/m ³	1.00x10 ⁻²	WHO (2000)
Limit value in drinking water	mg/m ³	5	WHO (1996)
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	WHO (2000)
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 ³	4.60x10 ⁻⁴	data VMM (1999, 2000)
Background indoor air	mg/m ³	4.60x10 ⁻⁴	 = outdoor air
Background drinking water	mg/m ³	5.00x10 ⁻²	 VMM (2006)

- a) Vinylchloride is a human carcinogen by all exposure routes. The carcinogenic effect is the most critical effect and was used to calculate the soil remediation values. In addition to the carcinogenic reference values, the S-Risk data sheet also provides the reference values for the non-carcinogenic effects of vinylchloride that were referenced in the background document to the soil remediation values.
- b) 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/m³. 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 m³/d.
- c) The original substance data sheet lists the reference values for carcinogenic non-threshold effects as a dose corresponding to an excess lifelong cancer risk of 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(dose at 1.10⁻⁵ (mg/kg.d)). In case of inhalation risks, the dose is first converted to a concentration by multiplying it with 70 kg (body weight) and dividing it by 20 m³/d (inhalation rate).


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 ³ /mol	296 (20°C)	Calculated
log Kow	g/g	1.94	Geometric mean
log Koc	dm ³ /kg	1.832381	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	3.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.8976 (25°C)	US-EPA (1996c)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵ (25°C)	US-EPA (1996c)
Kp	[cm/h]	1.66x10 ⁻¹	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	IARC (1999c) US-EPA (2001)
Systemic effects threshold ^{a)}			N not included in standard
TDI oral	mg/kg.d	1x10 ⁻²	US-EPA (2001)
TCL inhalation ^{b)}	mg/m ³	1x10 ⁻¹	ATSDR
TDI dermal	mg/kg.d	1x10 ⁻²	= oral value
Systemic effects no threshold			
Oral slope factor	(mg/kg.d) ⁻¹	1.5x10 ⁻³	WHO (1996)
inhalation unit risk ^{c)}	(mg/m ³) ⁻¹	2.3x10 ⁻²	US-EPA (2001)
Dermal slop factor	(mg/kg.d) ⁻¹	1.5x10 ⁻³	= oral value
Limit value in air	mg/m ³	4.00x10 ⁻⁴	US-EPA (2001)
Limit value in drinking water	mg/m ³	20	WHO (1996)? factor 10 difference
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 ³	1.50x10 ⁻⁴	Average from VMM (1999, 2000)
Background indoor air	mg/m ³	1.50x10 ⁻⁴	 = outdoor air
Background drinking water	mg/m ³	20	 VMM (2006)

- a) Trichloromethane is a human genotoxic carcinogen by all exposure routes. The carcinogenic effect is the most critical effect and was used to calculate the soil remediation values. In addition to the carcinogenic reference values, the S-Risk data sheet also provides reference values for the non-carcinogenic effects of vinylchloride. These values were selected from the values referenced in the background document to the soil remediation values.
- b) 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/m³. 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 m³/d.
- c) The original substance data sheet lists the reference values for carcinogenic non-threshold effects as a dose corresponding to an excess lifelong cancer risk of 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(dose at 1.10⁻⁵ (mg/kg.d)). In case of inhalation risks, the dose is first converted to a concentration by multiplying it with 70 kg (body weight) and dividing it by 20 m³/d (inhalation rate).

CHAPTER 5. SUBSTANCE DATA SHEETS CHLOROBENZENES

Data on substances that do not derive from the former substance data sheets are indicated with , accompanied with some explanation if appropriate. Detailed information on all new entries is given in Cornelis et al. (2013).

5.1. MONOCHLOROBENZENE

Parameter	Unit	Value	Source
CAS nr.		108-90-7	ATSDR (1990)
Type		organic	
Dissociating		no	
Molecular weight	g/mol	112.6	
Solubility	mg/l	500 (20°C)	Verschuieren (1983)
Vapour pressure	Pa	1173 (20°C)	Verschuieren (1983)
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	2.83	U.S.-EPA (1994b)
log Koc	dm ³ /kg	2.238046	U.S.-EPA (1994b)
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	3.5x10 ⁻⁶	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0.1	 = other chlorobenzenes
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	 values not searched for
BTF feed - egg	d/kg	0	 values not searched for
Carcinogenicity		assessed as non-carcinogen	?
Systemic effects threshold			
TDI oral	mg/kg.d	8.57x10 ⁻²	WHO (1993)
TCL inhalation ^{a)}	mg/m ³	3x10 ⁻¹	calculated from oral value
TDI dermal	mg/kg.d	8.57x10 ⁻¹	= oral value
averaging period	mg/m ³	1.30x10 ⁻¹	Hassauer et al. (1993)
Limit value in air	mg/m ³	300	WHO (1993)
Limit value in drinking water	mg/kg fw	-	
Limit value in plants			
Limit value in meat	mg/kg fw	-	

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	-	
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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

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 ³ /mol	-	
log Kow	g/g	3.1	Verschuieren (1983) Kile et al. (1995)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	2.00x10 ⁻⁶	van den Berg (1994), value 1,4-dichlorobenzene
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0.1	US-EPA (2004)
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	values not searched for
BTF feed - egg	d/kg	0	values not searched for
Carcinogenicity			
Systemic effects threshold		assessed as non-carcinogen	?
TDI oral	mg/kg.d	4.29x10 ⁻¹	WHO (1993)
TCL inhalation ^{a)}	mg/m ³	1.5	Calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	4.29x10 ⁻¹	= oral value
Limit value in air	mg/m ³	2.6x10 ⁻¹	Hassauer et al. (1993)
Limit value in drinking water	mg/m ³	1000	WHO (1993)
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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

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)	Verschueren (1983) Kühne et al. (1995)
Vapour pressure	Pa	200 (25°C)	Verschueren (1983)
Henry coefficient	Pa m ³ /mol	-	
log Kow	g/g	3.38	Verschueren (1983)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.00x10 ⁻⁶	van den Berg (1994), value 1,4-dichlorobenzene
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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		assessed as non-carcinogen	?
Systemic effects threshold			
TDI oral	mg/kg.d	4.29x10 ⁻¹	WHO (1993)
TCL inhalation ^{a)}	mg/m ³	1.5	Calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	4.29x10 ⁻¹	= oral value
Limit value in air	mg/m ³	0.26	Hassauer et al. (1993)
Limit value in drinking water	mg/m ³	1000	WHO (1993)
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		
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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

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	4.90×10^{-1} (22°C)	Verschueren (1983)
Vapour pressure	Pa	80 (20°C)	Verschueren (1983)
Henry coefficient	Pa m ³ /mol	-	
log Kow	g/g	3.46	Verschueren (1983) Mackay (1982)
log Koc	dm ³ /kg	2.689309	US-EPA (1994b) Kile et al. (1995)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.00×10^{-6}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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		assessed as non-carcinogen	?
Systemic effects threshold			
TDI oral	mg/kg.d	1.07×10^{-1}	WHO (1993)
TCL inhalation ^{a)}	mg/m ³	3.75×10^{-1}	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	1.07×10^{-1}	= oral value
Limit value in air	mg/m ³	8×10^{-1}	US-EPA, (1996a)
Limit value in drinking water	mg/m ³	300	WHO (1993)
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	

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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

5.5. 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 ³ /mol	calculated	
log Kow	g/g	4.03	US-EPA (1994b)
log Koc	dm ³ /kg	3.193403	US-EPA (1994b)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	1.00x10 ⁻⁶	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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		assessed as non-carcinogen	?
Systemic effects threshold			
TDI oral	mg/kg.d	7.7x10 ⁻³	WHO (1993)
TCL inhalation ^{a)}	mg/m ³	2.7x10 ⁻²	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	7.7x10 ⁻³	= oral TDI
Limit value in air	mg/m ³	9.00x10 ⁻³	Hassauer et al. (1993)
Limit value in drinking water	mg/m ³	20	WHO (1993)
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	

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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

5.6. 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 ³ /mol	-	
log Kow	g/g	4.6	Chiou (1985)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	1.00x10 ⁻⁶	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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		assessed as non-carcinogen	
Systemic effects threshold			
TDI oral	mg/kg.d	3x10 ⁻⁴	US-EPA (1991c)
TCL inhalation ^{a)}	mg/m ³	1x10 ⁻³	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	3x10 ⁻⁴	= oral value
Limit value in air	mg/m ³	-	
Limit value in drinking water	mg/m ³	9	calculated on the basis of the oral TDI
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	

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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.

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	5.60×10^{-1} (25°C)	Kühne et al. (1995)
Vapour pressure	Pa	0.133 (20°C)	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	5.19	Mackay (1982)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	1.00×10^{-6}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /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		assessed as non-carcinogen	?
Systemic effects threshold			
TDI oral	mg/kg.d	8×10^{-4}	US-EPA (1988b)
TCL inhalation ^{a)}	mg/m ³	3×10^{-3}	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	8×10^{-4}	= oral value
Limit value in air	mg/m ³	-	
Limit value in drinking water	mg/m ³	2.40	calculated on the basis of the oral TDI
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	

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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	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/m³. 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 m³/d.


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	1.13x10 ⁻²	Geometric mean
Vapour pressure	Pa	0.00187	Geometric mean
Henry coefficient	Pa m ³ /mol	47.5	calculated
log Kow	g/g	5.69	Geometric mean
log Koc	dm ³ /kg	4.692732	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	3.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.468	US-EPA (1996c)
Diffusion coefficient water (Dw)	m ² /d	5.04x10 ⁻⁵	US-EPA (1996c)
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00x10 ⁻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	IARC (2001) US-EPA (1996b)
Systemic effects threshold ^{a)}			N not in remediation value calculation
TDI oral	mg/kg.d	8x10 ⁻⁴	US-EPA (1996b)
TCL inhalation ^{b)}	mg/m ³	2.8x10 ⁻²	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	8x10 ⁻⁴	= oral value
Systemic effects no threshold			
Oral slope factor	(mg/kg.d) ⁻¹	3x10 ⁻¹	WHO (1996)
Inhalation unit risk ^{c)}	(mg/m ³) ⁻¹	4.6x10 ⁻¹	US-EPA (1996b)
Dermal slope factor	(mg/kg.d) ⁻¹	3x10 ⁻¹	= oral value
Limit value in air	mg/m ³	2.00x10 ⁻⁵	US-EPA (1996b)
Limit value in drinking water	mg/m ³	1	WHO (1996)
Limit value in plants	mg/kg fw	0.01 grain and tea 0.01: the rest	Detection limit
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 ³	1.00x10 ⁻⁶	conservative estimate WHO (1997)
Background indoor air	mg/m ³	1.00x10 ⁻⁶	= outdoor air
Background drinking water	mg/m ³	0	

- a) Trichloromethane is a human genotoxic carcinogen by all exposure routes. The carcinogenic effect is the most critical effect and was used to calculate the soil remediation values. In addition to the carcinogenic reference values, the S-Risk data sheet also provides reference values for the non-carcinogenic effects of vinylchloride. These values were selected from the values referenced in the background document to the soil remediation values.
- b) 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/m³. 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 m³/d.
- c) The original substance data sheet lists the reference values for carcinogenic non-threshold effects as a dose corresponding to an excess lifelong cancer risk of 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(dose at 1.10⁻⁵ (mg/kg.d)). In case of inhalation risks, the dose is first converted to a concentration by multiplying it with 70 kg (body weight) and dividing it by 20 m³/d (inhalation rate).

CHAPTER 6. SUBSTANCE DATA SHEETS CHLOROPHENOLS

Data on substances that do not derive from the former substance data sheets are indicated with , accompanied with some explanation if appropriate. Detailed information on all new entries is given in Cornelis et al. (2013).










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 ⁴ (25°C)	average
Vapour pressure	Pa	294 (25°C)	average
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	2.13	average
log Koc	dm ³ /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	5.00x10 ⁻⁹	Lijzen et al. (2001)
Dpvc	m ² /d	5.00x10 ⁻¹²	
Diffusion coefficient air (Da)	m ² /d	0.432	RAIS-online
Diffusion coefficient water (Dw)	m ² /d	8.18x10 ⁻⁵	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	5x10 ⁻³	IRIS (1993)
TCL inhalation ^{a)}	mg/m ³	1.75x10 ⁻²	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	5x10 ⁻³	= oral value

Parameter	Unit	Value	Source
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.75E-02	calculated on the basis of the oral TDI
Limit value in drinking water	mg/m ³	15	calculated on the basis of the TDI
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	Baars et al. (2001)
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 ³	0	Baars et al. (2001)
Background indoor air	mg/m ³	0	☒ = outdoor air
Background drinking water	mg/m ³	0	☒ no values

- 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/m³. 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 m³/d.

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 ³ (25°C)	average
Vapour pressure	Pa	25.5 (25°C)	average
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	3.08	average
log Koc	dm ³ /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	1.00x10 ⁻⁷	Lijzen et al. (2001)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.3	RAIS-online
Diffusion coefficient water (Dw)	m ² /d	7.58x10 ⁻⁵	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	3x10 ⁻³	IRIS (1988a)
TCL inhalation ^{a)}	mg/m ³	1.05x10 ⁻²	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	3x10 ⁻³	= oral TDI
averaging period		Child, adolescent, adult	
Limit value in air	mg/m ³	1.05x10 ⁻²	calculated on the basis of the oral TDI
Limit value in drinking water	mg/m ³	9	calculated on the basis of the TDI
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	Baars et al. (2001)
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 ³	0	Baars et al. (2001)
Background indoor air	mg/m ³	0	☒ = outdoor air
Background drinking water	mg/m ³	0	☒ no values

- 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/m³. 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 m³/d.

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 ³ (25°C)	average
Vapour pressure	Pa	4.77 (25°C)	average
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	3.72	average
log Koc	dm ³ /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	5.00x10 ⁻⁷	Lijzen et al. (2001)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.252	RAIS-online
Diffusion coefficient water (Dw)	m ² /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	1x10 ⁻¹	IRIS (1991b)
TCL inhalation ^{a)}	mg/m ³	3.5x10 ⁻¹	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	1x10 ⁻¹	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	3.50x10 ⁻¹	calculated on the basis of the oral TDI
Limit value in drinking water	mg/m ³	300	calculated on the basis of the TDI
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	Baars et al. (2001)
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 ³	0	Baars et al. (2001)
Background indoor air	mg/m ³	0	☒ = outdoor air
Background drinking water	mg/m ³	0	☒ no values

- 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/m³. 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 m³/d.

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 ² (25°C)	average
Vapour pressure	Pa	2.66	average
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	3.54	average
log Koc	dm ³ /kg	not used	dissociating
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	5.00x10 ⁻⁷	Lijzen et al. (2001)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.2736	RAIS-online
Diffusion coefficient water (Dw)	m ² /d	0.000054	RAIS-online
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.1	N RAIS-online
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 rapid screening did not provide values
BTF feed - egg	d/kg	0	N rapid screening did not provide values
Carcinogenicity		2B	IARC (1999a) (polychlorophenols)
Systemic effects threshold ^{a)}			N not included in standard
TDI oral	mg/kg.d	1x10 ⁻³	US-EPA (2007)
TCL inhalation ^{b)}	mg/m ³	3.5x10 ⁻³	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	1x10 ⁻³	= oral value
averaging period		child, adolescent, adult	
Systemic effects no threshold			
Oral slope factor	(mg/kg.d) ⁻¹	1.1x10 ⁻²	IRIS (1994a)
Inhalation unit risk ^{c)}	(mg/m ³) ⁻¹	3.1x10 ⁻³	IRIS (1994a)
Dermal slope factor	(mg/kg.d) ⁻¹	1.1x10 ⁻²	= oral value
Limit value in air	mg/m ³	3.00x10 ⁻³	IRIS (1994a)
Limit value in drinking water	mg/m ³	200	WHO (1993)
Limit value in plants	mg/kg fw		
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	Baars et al. (2001)
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 ³	0	Baars et al. (2001)
Background indoor air	mg/m ³	0	 = outdoor air
Background drinking water	mg/m ³	0	 No values

- a) 2,4,6-Trichlorophenol is a genotoxic carcinogen by all exposure routes and the carcinogenic reference values were used when calculating soil remediation values. These data were taken over in the S-Risk substance data sheet. In addition to this, data for the non-carcinogenic effects of 2,4,6-trichlorophenol were searched for and added to the S-Risk substance data sheet.
- b) 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/m³. 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 m³/d.
- c) The original substance data sheet lists the reference values for carcinogenic non-threshold effects as a dose corresponding to an excess lifelong cancer risk of 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(dose at 1.10⁻⁵ (mg/kg.d)). In case of inhalation risks, the dose is first converted to a concentration by multiplying it with 70 kg (body weight) and dividing it by 20 m³/d (inhalation rate).

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 ² (25°C)	average
Vapour pressure	Pa	0.64	average
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	4.32	average
log Koc	dm ³ /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	1.00x10 ⁻⁶	Lijzen et al. (2001)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.18744	RAIS-online
Diffusion coefficient water (Dw)	m ² /d	6.14x10 ⁻⁵	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	3x10 ⁻²	US-EPA (1992)
TCL inhalation ^{a)}	mg/m ³	1.05x10 ⁻¹	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	3x10 ⁻²	= oral value
averaging period			
Limit value in air	mg/m ³	1.05x10 ⁻¹	calculated on the basis of the oral TDI
Limit value in drinking water	mg/m ³	90	calculated on the basis of the TDI
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	Baars et al. (2001)
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 ³	0	Baars et al. (2001)
Background indoor air	mg/m ³	0	☒ = outdoor air
Background drinking water	mg/m ³	0	☒ no values

- 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/m³. 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 m³/d.

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 ³ /mol	calculated	
log Kow	g/g	4.81	average
log Koc	dm ³ /kg	not used	dissociating
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	2.24x10 ⁻⁶	Lijzen et al. (2001)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.48	RAIS-online
Diffusion coefficient water (Dw)	m ² /d	5.28x10 ⁻⁵	RAIS-online
Kp	[cm/h]	calculated	
FA	-	0.9	US-EPA, 2004
ABS dermal soil/dust	-	2.50x10 ⁻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 ^{a)}			not part of calculation of remediation values
TDI oral	mg/kg.d	5x10 ⁻³	US-EPA (2010)
TCL inhalation ^{b)}	mg/m ³	1.75x10 ⁻²	calculated on the basis of the oral TDI
TDI dermal	mg/kg.d	5x10 ⁻³	= oral value
averaging period		child, adolescent, adult	
Systemische effecten geen drempel			
Oral slope factor	(mg/kg.d) ⁻¹	1.1x10 ⁻¹	US-EPA IRIS (1993) – no longer available
Inhalation unit risk ^{c)}	(mg/m ³) ⁻¹	3.2x10 ⁻²	calculated on the basis of the oral TDI
Dermal slope factor	(mg/kg.d) ⁻¹	1.1x10 ⁻¹	= oral value
Limit value in air	mg/m ³	-	
Limit value in drinking water	mg/m ³	9	WHO (1998)
Limit value in plants	mg/kg fw	0.01 (all plants)	EC (2005)

Parameter	Unit	Value	Source
Limit value in meat			N
Beef	mg/kg fw	0.01	EC (2005)
Mutton	mg/kg fw	0.01	EC (2005)
Liver	mg/kg fw	0.01	EC (2005)
Kidney	mg/kg fw	0.01	EC (2005)
Milk	mg/kg fw	0.01	EC (2005)
Butter	mg/kg fw	0.01	EC (2005)
Egg	mg/kg fw	0.01	EC (2005)
Dietary background adults	mg/kg day	1.00×10^{-6}	Baars et al. (2001)
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	N Cornelis et al. (2013)
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 ³	6.80×10^{-6}	Baars et al. (2001)
Background indoor air	mg/m ³	6.80×10^{-6}	N = outdoor air
Background drinking water	mg/m ³	0	N no values

- a) Pentachlorophenol is a genotoxic carcinogen by all exposure routes and the carcinogenic reference values were used when calculating soil remediation values. These data were taken over in the S-Risk substance data sheet. In addition to this, data for the non-carcinogenic effects of 2,4,6-trichlorophenol were searched for and added to the S-Risk substance data sheet.
- b) 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/m³. 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 m³/d.
- c) The original substance data sheet lists the reference values for carcinogenic non-threshold effects as a dose corresponding to an excess lifelong cancer risk of 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = $1.10^{-5}/(\text{dose at } 1.10^{-5} \text{ (mg/kg.d)})$. In case of inhalation risks, the dose is first converted to a concentration by multiplying it with 70 kg (body weight) and dividing it by 20 m³/d (inhalation rate).

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