

Final report

S-Risk for the Walloon region - substance data sheets part 2: BTEX, styrene, phenol and trimethylbenzenes

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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

Date	Modification

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/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 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, Bierkens, and Standaert, 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, chlorobenzenes 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 2. SUBSTANCE DATA SHEETS BTEX, STYRENE AND PHENOL

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.

2.1. BENZENE

Parameter	Unit	Value	Source
CAS nr.		71-43-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	78.11	
Solubility	mg/l	1777 (25°C)	average
Vapour pressure*	Pa	12516 (25°C)	average
Henry coefficient	Pa m ³ /mol	552 (25°C)	average
log Kow	g/g	2.13	Geometric mean
log Koc	dm ³ /kg	1.9	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	1.4x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.74	average
Diffusion coefficient water (Dw)	m ² /d	9.07x10 ⁻⁵	average
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0	N considered negligible
BTF beef	d/kg	calculated	N
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
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		1 A	W IARC (2012) W US-EPA (2000)
Systemic effects threshold			
TDI oral	mg/kg.d	5.0x10 ⁻⁴	ATSDR (2007)
TCA inhalation	mg/m ³	3.0x10 ⁻³	OEHHA (2014)
TDI dermal	mg/kg.d	5.0x10 ⁻⁴	= oral value
Systemic effects non-threshold			

Parameter	Unit	Value	Source
Oral slope factor	(mg/kg.d) ⁻¹	5.5x10 ⁻²	W US-EPA (2000)
Inhalation unit risk	(mg/m ³) ⁻¹	6.0x10 ⁻³	WHO (2000)
Dermal slope factor	(mg/kg.d) ⁻¹	5.5x10 ⁻²	W = oral value
Limit in outdoor air	mg/m ³	5.00x10 ⁻³	W EC (2008); AGW (2010)
Limit value in drinking water	mg/m ³	1.0	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	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	W
Background root crops	mg/kg fw	0	W
Background bulbous plants (onion ...)	mg/kg fw	0	W
Background fruit vegetables	mg/kg fw	0	W
Background cabbage	mg/kg fw	0	W
Background leafy vegetables	mg/kg fw	0	W
Background legume	mg/kg fw	0	W
Background beef	mg/kg fw	0	W
Background offal	mg/kg fw	0	W
Background milk	mg/kg fw	0	W
Background butter	mg/kg fw	0	W
Background eggs	mg/kg fw	0	W
Background outdoor air	mg/m ³	0	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	W

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

2.2. TOLUENE

Parameter	Unit	Value	Source
CAS nr.		108-88-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	92.13	
Solubility	mg/l	523 (25°C)	average
Vapour pressure*	Pa	3802 (25°C)	average
Henry coefficient	Pa m ³ /mol	655 (25°C)	average
log Kow	g/g	2.65	Geometric mean
log Koc	dm ³ /kg	2.12	Geometric mean
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	1.2x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.6936	average
Diffusion coefficient water (Dw)	m ² /d	7.66x10 ⁻⁵	average
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	3.00x10 ⁻²	US-EPA (1995, 2003b)
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 D	IARC (1999a) US-EPA (2005)
Systemic effects threshold			
TDI oral	mg/kg.d	8.0x10 ⁻²	US-EPA (2005)
TCL inhalation	mg/m ³	2.6x10 ⁻¹	WHO (2000)
TDI dermal	mg/kg.d	8.0x10 ⁻²	= oral TDI
averaging period		Child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	
Limit value in drinking water	mg/m ³	-	
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	W
Background root crops	mg/kg fw	0	W
Background bulbous plants (onion ...)	mg/kg fw	0	W
Background fruit vegetables	mg/kg fw	0	W
Background cabbage	mg/kg fw	0	W
Background leafy vegetables	mg/kg fw	0	W
Background legume	mg/kg fw	0	W
Background beef	mg/kg fw	0	W
Background offal	mg/kg fw	0	W
Background milk	mg/kg fw	0	W
Background butter	mg/kg fw	0	W
Background eggs	mg/kg fw	0	W
Background outdoor air	mg/m ³	0	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	

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

2.3. ETHYLBENZENE

Parameter	Unit	Value	Source
CAS nr.		100-41-4	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	106.2	
Solubility	mg/l	165 (25°C)	average
Vapour pressure*	Pa	1280 (25°C)	average
Henry coefficient	Pa m ³ /mol	788 (25°C)	average
log Kow	g/g	3.15	Geometric mean
log Koc	dm ³ /kg	2.3	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.1x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.6168	average
Diffusion coefficient water (Dw)	m ² /d	7.18x10 ⁻⁵	average
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	3.00x10 ⁻²	N US-EPA (1995, 2003b)
BTF beef	d/kg	calculated	N
BTF mutton	d/kg	calculated	
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 D	W IARC (2000) US-EPA (1991)
Systemic effects threshold			
TDI oral	mg/kg.d	9.70x10 ⁻²	WHO (2000); ATSDR (2010); US-EPA (2008)
TCL inhalation	mg/m ³	3.0 x10 ⁻¹	W ATSDR (2010)
TDI dermal	mg/kg.d	9.70x10 ⁻²	W = oral TDI
averaging period		child, adolescent, adult	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) ⁻¹	1.1x10 ⁻²	W OEHHA (2009)
Inhalation unit risk	(mg/m ³) ⁻¹	2.5x10 ⁻³	W OEHHA (2007)
Dermal slope factor	(mg/kg.d) ⁻¹	1.1x10 ⁻²	W = oral value
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	W
Background root crops	mg/kg fw	0	W
Background bulbous plants (onion ...)	mg/kg fw	0	W
Background fruit vegetables	mg/kg fw	0	W
Background cabbage	mg/kg fw	0	W
Background leafy vegetables	mg/kg fw	0	W
Background legume	mg/kg fw	0	W
Background beef	mg/kg fw	0	W
Background offal	mg/kg fw	0	W
Background milk	mg/kg fw	0	W
Background butter	mg/kg fw	0	W
Background eggs	mg/kg fw	0	W
Background outdoor air	mg/m ³	0	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	W

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

2.4. O-XYLENE

Parameter	Unit	Value	Source
CAS nr.		95-47-6	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	106.2	
Solubility	mg/l	186 (25°C)	average
Vapour pressure*	Pa	889 (25°C)	average
Henry coefficient	Pa m ³ /mol	548 (25°C)	average
log Kow	g/g	3.07	Geometric mean
log Koc	dm ³ /kg	2.15	Geometric mean
Log Koa	g/g	calculated	W
BCF		calculated	
Dpe	m ² /d	1.6x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.7512	average
Diffusion coefficient water (Dw)	m ² /d	7.73x10 ⁻⁵	average
Kp	[cm/h]	calculated	W
FA	-	1	W
ABS dermal soil/dust	-	3.00x10 ⁻²	W US-EPA (1995, 2003b)
BTF beef	d/kg	calculated	W
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	W
BTF kidney	d/kg	calculated	W
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	W values not searched for
BTF feed - egg	d/kg	0	W values not searched for
Carcinogenicity		3 D	IARC (1999a) US-EPA IRIS date not found, before 2002
Systemic effects threshold			
TDI oral	mg/kg.d	2.0x10 ⁻¹	W ATSDR (2003) ; US-EPA (2003a)
TCL inhalation	mg/m ³	1.0x10 ⁻¹	W US-EPA (2003a)
TDI dermal	mg/kg.d	2.0x10 ⁻¹	W = oral value
averaging period		child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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

BTEX, styrene, phenol and trimethylbenzenes

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

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

2.5. M-XYLENE

Parameter	Unit	Value	Source
CAS nr.		108-38-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	106.2	
Solubility	mg/l	166 (25°C)	average
Vapour pressure*	Pa	1121 (25°C)	average
Henry coefficient	Pa m ³ /mol	710 (25°C)	average
log Kow	g/g	3.18	Geometric mean
log Koc	dm ³ /kg	2.29	Geometric mean
Log Koa	g/g	-	W
BCF		calculated	
Dpe	m ² /d	1.6x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.5952	average
Diffusion coefficient water (Dw)	m ² /d	6.74x10 ⁻⁵	average
Kp	[cm/h]	calculated	W
FA	-	1	W
ABS dermal soil/dust	-	3.00x10 ⁻²	W US-EPA (1995, 2003b)
BTF beef	d/kg	calculated	W
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	W
BTF kidney	d/kg	calculated	W
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	W values not searched for
BTF feed - egg	d/kg	0	W values not searched for
Carcinogenicity		3 D	IARC (1999a) US-EPA IRIS date not found, before 2002
Systemic effects threshold			
TDI oral	mg/kg.d	2.0x10 ⁻¹	W ATSDR (2003) ; US-EPA (2003a)
TCL inhalation	mg/m ³	1.0x10 ⁻¹	W US-EPA (2003a)
TDI dermal	mg/kg.d	2.0x10 ⁻¹	W = oral value
averaging period		Child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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

BTEX, styrene, phenol and trimethylbenzenes

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

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

2.6. P-XYLENE

Parameter	Unit	Value	Source
CAS nr.		106-42-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	106.2	
Solubility	mg/l	179 (25°C)	average
Vapour pressure*	Pa	1173 (25°C)	average
Henry coefficient	Pa m ³ /mol	713 (25°C)	average
log Kow	g/g	3.16	Geometric mean
log Koc	dm ³ /kg	2.47	Geometric mean
Log Koa	g/g	calculated	W
BCF		calculated	
Dpe	m ² /d	1.6x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.6648	average
Diffusion coefficient water (Dw)	m ² /d	7.06x10 ⁻⁵	average
Kp	[cm/h]	calculated	W
FA	-	1	W
ABS dermal soil/dust	-	3.00x10 ⁻²	W US-EPA (1995, 2003b)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	W
BTF liver	d/kg	calculated	W
BTF kidney	d/kg	calculated	W
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	W values not searched for
BTF feed - egg	d/kg	0	W values not searched for
Carcinogenicity		3 D	IARC (1999a) US-EPA IRIS date not found, before 2002
Systemic effects threshold			
TDI oral	mg/kg.d	2.0x10 ⁻¹	W ATSDR (2003) ; US-EPA (2003a)
TCL inhalation	mg/m ³	1.0x10 ⁻¹	W US-EPA (2003a)
TDI dermal	mg/kg.d	2.0x10 ⁻¹	W = oral value
averaging period		child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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

BTEX, styrene, phenol and trimethylbenzenes

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

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

2.7. STYRENE

Parameter	Unit	Value	Source
CAS nr.		9003-53-6	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	104.51	
Solubility	mg/l	272 (25°C)	average
Vapour pressure*	Pa	850 (25°C)	average
Henry coefficient	Pa m ³ /mol	271 (25°C)	average
log Kow	g/g	2.97	Geometric mean
log Koc	dm ³ /kg	2.86	Geometric mean
Log Koa	g/g	calculated	W
BCF		calculated	
Dpe	m ² /d	2x10 ⁻⁶	van den Berg (1995)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.6144	average
Diffusion coefficient water (Dw)	m ² /d	6.96x10 ⁻⁵	average
Kp	[cm/h]	calculated	W
FA	-	1	W
ABS dermal soil/dust	-	3.00x10 ⁻²	W US-EPA (1995, 2003b)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	W
BTF liver	d/kg	calculated	
BTF kidney	d/kg	calculated	
BTF milk	d/kg	calculated	W
BTF soil – egg	d/kg	0	W values not searched for
BTF feed - egg	d/kg	0	W values not searched for
Carcinogenicity		2B	IARC (2002)
Systemic effects threshold			
TDI oral	mg/kg.d	2.0x10 ⁻¹	W US-EPA (1990)
TCL inhalation	mg/m ³	1.0x10 ⁻¹	W Vermont (2007)
TDI dermal	mg/kg.d	2.0x10 ⁻¹	W = oral value
averaging period		child, adolescent, lifelong	
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) ⁻¹	1.0x10 ⁻⁸	W dummy value (considered non carcinogenic by oral exposure)
Inhalation unit risk	(mg/m ³) ⁻¹	5.7x10 ⁻⁴	W New Jersey (2009)
Dermal slope factor	(mg/kg.d) ⁻¹	1.0x10 ⁻⁸	W = oral value
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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	W
Dietary background children	mg/kg.day	0	W
Background potatoes	mg/kg fw	0	W
Background root crops	mg/kg fw	0	W
Background bulbous plants (onion ...)	mg/kg fw	0	W
Background fruit vegetables	mg/kg fw	0	W
Background cabbage	mg/kg fw	0	W
Background leafy vegetables	mg/kg fw	0	W
Background legume	mg/kg fw	0	W
Background beef	mg/kg fw	0	W
Background offal	mg/kg fw	0	W
Background milk	mg/kg fw	0	W
Background butter	mg/kg fw	0	W
Background eggs	mg/kg fw	0	W
Background outdoor air	mg/m ³	0	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	W

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

2.8. PHENOL (W)

Parameter	Unit	Value	Source
CAS nr.		108-95-2	
Type		organic	
Dissociating		yes	
Acid dissociation		Yes	
pKa		10	Lijzen, et al. (2001)
Molecular weight	g/mol	94.11	
Solubility	mg/l	82000 (15°C)	Verschuieren (1996)
Vapour pressure	Pa	46.3 (10°C)	Geometric mean
Henry coefficient	Pa m ³ /mol	0.0761 (25°C)	Sander (1999) – Geometric mean
log Kow	g/g	1.47	Lijzen, et al. (2001)
log Koc	dm ³ /kg	1.52	Lijzen, et al. (2001)
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	8.4x10 ⁻⁹	Lijzen, et al. (2001)
Dpvc	m ² /d	8.4x10 ⁻¹²	
Diffusion coefficient air (Da)	m ² /d	0.7776	CSOIL formula : Da (m ² /h) = 0,036*(76/M) ^{0,5}
Diffusion coefficient water (Dw)	m ² /d	7.776x10 ⁻⁵	CSOIL formula : Dw (m ² /h) = 3,6e-6*(76/M) ^{0,5}
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	0.1	
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 D	IARC (1999b) US-EPA (2002)
Systemic effects threshold			
TDI oral	mg/kg.d	4.0x10 ⁻²	Baars, et al. (2001)
TCL inhalation	mg/m ³	2.0x10 ⁻²	Baars, et al. (2001)
TDI dermal	mg/kg.d	4.0x10 ⁻²	= oral value
averaging period		child, adolescent, lifelong	
Limit in outdoor air	mg/m ³	-	
Limit value in drinking water	mg/m ³	-	
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 ³	0	
Background indoor air	mg/m ³	0	
Background drinking water	mg/m ³	0	

CHAPTER 3. SUBSTANCE DATA SHEETS TRIMETHYLBENZENES

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.

3.1. 1,2,3-TRIMETHYLBENZENE

Parameter	Unit	Value	Source
CAS nr.		526-73-8	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	120.2	Geometric mean
Solubility	mg/l	67.4 (25°C)	Geometric mean
Vapour pressure*	Pa	225 (25°C)	Geometric mean
Henry coefficient	Pa m ³ /mol	401 (25°C)	Calculated from S and P
log Kow ^{a)}	g/g	3.6 (25°C)	Geometric mean
log Koc	dm ³ /kg	2.836957	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	6.4x10 ⁻⁶	van den Berg (1997)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.696 (25°C)	Calculated value
Diffusion coefficient water (Dw)	m ² /d	6.86x10 ⁻⁵ (25°C)	Calculated value
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.1	N semi-volatile chemical (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		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	5x10 ⁻²	CEHT (2001)
TCL inhalation	mg/m ³	9.8x10 ⁻³	Vermont (2007)
TDI dermal	mg/kg.d	5x10 ⁻²	N = oral value
averaging period		Child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	W

Parameter	Unit	Value	Source
Limit value in drinking water	mg/m ³	-	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	
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	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	

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

a) The original substance data sheet from the background document for soil remediation values mentions $K_{ow} = 3.6$. The correct value is $\log K_{ow} = 3.6$. The latter value was used in the calculation of clean-up values and is also used in the Vlier-Humaan model.

3.2. 1,2,4-TRIMETHYLBENZENE

Parameter	Unit	Value	Source
CAS nr.		95-63-6	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	120.2	
Solubility	mg/l	62.2 (25°C)	Geometric mean
Vapour pressure*	Pa	225 (25°C)	Geometric mean
Henry coefficient	Pa m ³ /mol	631 (25°C)	Calculated from S and P
log Kow ^{a)}	g/g	3.6 (25°C)	Geometric mean
log Koc	dm ³ /kg	3.106871	Geometric mean
Log Koa	g/g	calculated	W
BCF		calculated	
Dpe	m ² /d	6.4x10 ⁻⁶	van den Berg (1997)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.6864 (25°C)	Calculated value
Diffusion coefficient water (Dw)	m ² /d	6.86x10 ⁻⁵ (25°C)	Calculated value
Kp	[cm/h]	calculated	W
FA	-	1	W
ABS dermal soil/dust	-	0.1	W semi-volatile chemical (US-EPA, 2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	W
BTF liver	d/kg	calculated	W
BTF kidney	d/kg	calculated	W
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	W values not searched for
BTF feed - egg	d/kg	0	W values not searched for
Carcinogenicity		D	US-EPA (non-traceable)
Systemic effects threshold			
TDI oral	mg/kg.d	0.05	CEHT (2001)
TCL inhalation	mg/m ³	9.8x10 ⁻³	Vermont (2007)
TDI dermal	mg/kg.d	0.05	W = oral value
averaging period		child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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 ³	0	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	

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

a) The original substance data sheet from the background document for soil remediation values mentions $K_{ow} = 3.6$. The correct value is $\log K_{ow} = 3.6$. The latter value was used in the calculation of clean-up values and is also used in the Vlier-Humaan model.

3.3. 1,3,5-TRIMETHYLBENZENE

Parameter	Unit	Value	Source
CAS nr.		108-67-8	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	120.2	
Solubility	mg/l	67.6 (25°C)	Geometric mean
Vapour pressure*	Pa	326 (25°C)	Geometric mean
Henry coefficient	Pa m ³ /mol	774 (25°C)	Calculated from S and P
log Kow ^{a)}	g/g	3.7 (25°C)	Geometric mean
log Koc	dm ³ /kg	2.832509	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	6.4E-06	van den Berg (1997)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.6864 (25°C)	calculated value
Diffusion coefficient water (Dw)	m ² /d	6.86x10 ⁻⁵ (25°C)	calculated value
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	0.1	N semi-volatile chemical (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	US-EPA (cannot be traced back)
Systemic effects threshold			
TDI oral	mg/kg.d	0.05	CEHT (2001)
TCL inhalation	mg/m ³	9.8x10 ⁻³	Vermont (2007)
TDI dermal	mg/kg.d	0.05	N = oral value
averaging period		child, adolescent, adult	
Limit in outdoor air	mg/m ³	-	W
Limit value in drinking water	mg/m ³	-	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	

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	W
Background indoor air	mg/m ³	0	W
Background drinking water	mg/m ³	0	

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

a) The original substance data sheet from the background document for soil remediation values mentions $K_{ow} = 3.6$. The correct value is $\log K_{ow} = 3.6$. The latter value was used in the calculation of clean-up values and is also used in the Vlier-Humaan model.

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