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Final report

S-Risk substance data sheets – Part 2: BTEX, styrene 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
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

04/11/2013	p-xylene: the limit in air was erroneously listed as the limit in drinking water whereas the limit in drinking water was listed under the limit for vegetables; this has been corrected
07/02/2017	Typos corrected

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 formely used parameters to calculate dermal absorption, namely the fraction adsorbed for dermal uptake via soil and dust, and the dermal permeability coefficient for dermal uptake from water. The latter parameter is combined with a parameter FA.
- **Bioconcentration factors plants (BCF)**: For metals and arsenic very often either the BCF for maize or the BCF for grass was missing. In these cases the same BCF was used for maize and grass. Because this is incorrect, there is a need to search for additional BCFs.
- **Bioconcentration factors plants (BCF):** for organic compounds plant uptake in S-Risk can either be calculated starting from substance- and plant-specific characteristics or directly from BCF values expressed in mg/kg dm in the plant per mg/m^3 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 the 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 1,1,1-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 for benzo(a)pyrene and dibenz(a,h)antracene;
- 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, and Standaert, 2013a). 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 polycylic 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 AND STYRENE

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. (2013a).

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 m³/mol	552 (25°C)	average
log Kow	g/g	2.13	Geometric mean
log Koc	dm³/kg	1.9	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	$1.4x10^{-6}$	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.74	average
Diffusion coefficient water (Dw)	m²/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	IARC (1999b) US-EPA (2000a)
Systemic effects threshold[a)]			N (not accounted for in the calculation of the Vlarebo values)
TDI oral	mg/kg.d	$5x10^{-4}$	ATSDR (2007)
TCA inhalation	mg/m³	$9.6x10^{-3}$	ATSDR (2007)
TDI dermal	mg/kg.d	$5x10^{-4}$	= oral value

Parameter	Unit	Value	Source
Systemic effects no threshold[b)]			
Oral slope factor	$(mg/kg.d)^{-1}$	0.0303	WHO (1996)
Inhalation unit risk	$(mg/m^3)^{-1}$	0.006	WHO (2000)
Dermal slope factor	$(mg/kg.d)^{-1}$	0.0303	N = oral value
Limit in air	mg/m^3	$5.00x10^{-3}$	EC ("Richtlijn 2000/69/EG van het Europees Parlement en de Raad van 16 november 2000 betreffende grenswaarden voor benzeen en koolstofmonoxide in de lucht," 2000)
Limit value in drinking water	mg/m^3	10	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	$3.40x10^{-5}$	MAFF (1995)
Dietary background children	mg/kg.day	relative to adults (cfr. TGD)	N Cornelis et al. (2013b)
Background potatoes	mg/kg fw	0.001	MAFF (1995)
Background root crops	mg/kg fw	0.001	MAFF (1995)
Background bulbous plants (onion …)	mg/kg fw	0.001	MAFF (1995)
Background fruit vegetables	mg/kg fw	0.001	MAFF (1995)
Background cabbage	mg/kg fw	0.001	MAFF (1995)
Background leafy vegetables	mg/kg fw	0.001	MAFF (1995)
Background legume	mg/kg fw	0.001	MAFF (1995)
Background beef	mg/kg fw	0.005	MAFF (1995)
Background offal	mg/kg fw	0.006	MAFF (1995)
Background milk	mg/kg fw	0.001	MAFF (1995)
Background butter	mg/kg fw	0.001	MAFF (1995)
Background eggs	mg/kg fw	0.001	N MAFF (1995)
Background outdoor air	mg/m^3	$1.60x10^{-3}$	VMM (1998)
Background indoor air	mg/m^3	$1.60x10^{-3}$	N = outdoor air
Background drinking water	mg/m^3	$1.00x10^{-1}$	N VMM (2006)

[a)] When calculating clean-up values, only the most critical effect – being cancer - was accounted for. To illustrate the S-Risk approach, values for systemic threshold effects were searched for and added to the S-Risk database.

[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 $1/10^5$. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor $((mg/kg.d)^{-1}) = 1.10^{-5}/(\text{dose at } 1.10^{-5} (mg/kg.d))$. 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 m^3/d (inhalation rate).

2.2. TOLUENE

Parameter	Unit	Value	Source
CAS nr.		3108-88-3	
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 m³/mol	655 (25°C)	average
log Kow	g/g	2.65	Geometric mean
log Koc	dm³/kg	2.12	Geometric mean
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m²/d	$1.2x10^{-6}$	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.6936	average
Diffusion coefficient water (Dw)	m²/d	$7.66x10^{-5}$	average
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	$3.00x10^{-2}$	N US-EPA (1995, 2003)
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	IARC (1999a) US-EPA (2000b)
Systemic effects threshold			
TDI oral	mg/kg.d	$2.23x10^{-1}$	WHO (1996)
TCL inhalation[a)]	mg/m³	$2.6x10^{-1}$	WHO (2000)
TDI dermal	mg/kg.d	$2.23x10^{-1}$	N = oral TDI
averaging period		Child, adolescent, adult	
Limit in air	mg/m³	$2.60x10^{-1}$	WHO (2000)
Limit value in drinking water	mg/m³	700	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	$1.10x10^{-4}$	MAFF (1995)
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	N Cornelis et al. (2013b)

Parameter	Unit	Value	Source
Background potatoes	mg/kg fw	0.003	MAFF (1995)
Background root crops	mg/kg fw	0.003	MAFF (1995)
Background bulbous plants (onion …)	mg/kg fw	0.003	MAFF (1995)
Background fruit vegetables	mg/kg fw	0.002	MAFF (1995)
Background cabbage	mg/kg fw	0.002	MAFF (1995)
Background leafy vegetables	mg/kg fw	0.003	MAFF (1995)
Background legume	mg/kg fw	0.002	MAFF (1995)
Background beef	mg/kg fw	0.014	MAFF (1995)
Background offal	mg/kg fw	0.014	MAFF (1995)
Background milk	mg/kg fw	0.004	MAFF (1995)
Background butter	mg/kg fw	0.02	MAFF (1995)
Background eggs	mg/kg fw	0.007	" MAFF (1995)
Background outdoor air	mg/m³	$4.20.10^{-3}$	Calculated from VMM (1999, 2000)
Background indoor air	mg/m³	$4.20.10^{-3}$	" = outdoor air
Background drinking water	mg/m³	0	No values for Flanders

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.

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 m³/mol	788 (25°C)	average
log Kow	g/g	3.15	Geometric mean
log Koc	dm³/kg	2.3	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	2.1×10^{-6}	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.6168	average
Diffusion coefficient water (Dw)	m²/d	7.18×10^{-5}	average
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	3.00×10^{-2}	N US-EPA (1995, 2003)
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		3 D	IARC (2000) US-EPA (1991)
Systemic effects threshold			
TDI oral	mg/kg.d	9.71×10^{-2}	WHO (1996)
TCL inhalation[a)]	mg/m³	22	WHO (2000)
TDI dermal	mg/kg.d	9.71×10^{-2}	N = orale TDI
averaging period		child, adolescent, adult	
Limit in air	mg/m³	22	WHO (2000)
Limit value in drinking water	mg/m³	300	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	6.00×10^{-5}	MAFF (1995)
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	N Cornelis et al. (2013b)

Parameter	Unit	Value	Source
Background potatoes	mg/kg fw	0.002	MAFF (1995)
Background root crops	mg/kg fw	0.002	MAFF (1995)
Background bulbous plants (onion …)	mg/kg fw	0.002	MAFF (1995)
Background fruit vegetables	mg/kg fw	0.002	MAFF (1995)
Background cabbage	mg/kg fw	0.002	MAFF (1995)
Background leafy vegetables	mg/kg fw	0.002	MAFF (1995)
Background legume	mg/kg fw	0.002	MAFF (1995)
Background beef	mg/kg fw	0.004	MAFF (1995)
Background offal	mg/kg fw	0.003	MAFF (1995)
Background milk	mg/kg fw	0.002	MAFF (1995)
Background butter	mg/kg fw	0.002	MAFF (1995)
Background eggs	mg/kg fw	0.002	MAFF (1995)
Background outdoor air	mg/m³	8.00×10^{-4}	Calculated from VMM (1999, 2000)
Background indoor air	mg/m³	8.00×10^{-4}	= outdoor air
Background drinking water	mg/m³	0	no values for Flanders

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.

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 m³/mol	548 (25°C)	average
log Kow	g/g	3.07	Geometric mean
log Koc	dm³/kg	2.15	Geometric mean
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m²/d	1.6×10^{-6}	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.7512	average
Diffusion coefficient water (Dw)	m²/d	7.73×10^{-5}	average
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	3.00×10^{-2}	US-EPA (1995, 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	0	values not searched for
BTF feed - egg	d/kg	0	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	1.79×10^{-1}	WHO (1996)
TCL inhalation[a)]	mg/m³	8.7×10^{-1}	WHO (2000)
TDI dermal	mg/kg.d	1.79×10^{-1}	= oral value
averaging period		child, adolescent, adult	
Limit in air	mg/m³	8.70×10^{-1}	WHO (2000)
Limit value in drinking water	mg/m³	500	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	6.60×10^{-5}	MAFF (1995)

Parameter	Unit	Value	Source
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	Cornelis et al. (2013b)
Background potatoes	mg/kg fw	0.004	MAFF (1995)
Background root crops	mg/kg fw	0.004	MAFF (1995)
Background bulbous plants (onion …)	mg/kg fw	0.004	MAFF (1995)
Background fruit vegetables	mg/kg fw	0.002	MAFF (1995)
Background cabbage	mg/kg fw	0.002	MAFF (1995)
Background leafy vegetables	mg/kg fw	0.002	MAFF (1995)
Background legume	mg/kg fw	0.002	MAFF (1995)
Background beef	mg/kg fw	0.005	MAFF (1995)
Background offal	mg/kg fw	0.002	MAFF (1995)
Background milk	mg/kg fw	0.002	MAFF (1995)
Background butter	mg/kg fw	0.002	MAFF (1995)
Background eggs	mg/kg fw	0.002	MAFF (1995)
Background outdoor air	mg/m³	9.00×10^{-4}	Calculated from VMM (1999, 2000)
Background indoor air	mg/m³	9.00×10^{-4}	= outdoor air
Background drinking water	mg/m³	3.33×10^{-2}	VMM (2006) – value for xylene divided by 3

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.

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 m³/mol	710 (25°C)	average
log Kow	g/g	3.18	Geometric mean
log Koc	dm³/kg	2.29	Geometric mean
Log Koa	g/g	-	
BCF		calculated	
Dpe	m²/d	$1.6x10^{-6}$	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.5952	average
Diffusion coefficient water (Dw)	m²/d	$6.74x10^{-5}$	average
Kp	[cm/h]	calculated	
FA	-	1	
ABS dermal soil/dust	-	$3.00x10^{-2}$	US-EPA (1995, 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	0	values not searched for
BTF feed - egg	d/kg	0	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	$1.79x10^{-1}$	WHO (1996)
TCL inhalation[a)]	mg/m³	$8.7x10^{-1}$	WHO (2000)
TDI dermal	mg/kg.d	$1.79x10^{-1}$	= oral value
averaging period		Child, adolescent, adult	
Limit in air	mg/m³	$8.70x10^{-1}$	WHO (2000)
Limit value in drinking water	mg/m³	500	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	$7.00x10^{-5}$	MAFF (1995)

Parameter	Unit	Value	Source
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	Cornelis et al. (2013b)
Background potatoes	mg/kg fw	0.002	MAFF (1995)
Background root crops	mg/kg fw	0.002	MAFF (1995)
Background bulbous plants (onion …)	mg/kg fw	0.002	MAFF (1995)
Background fruit vegetables	mg/kg fw	0.002	MAFF (1995)
Background cabbage	mg/kg fw	0.002	MAFF (1995)
Background leafy vegetables	mg/kg fw	0.002	MAFF (1995)
Background legume	mg/kg fw	0.002	MAFF (1995)
Background beef	mg/kg fw	0.007	MAFF (1995)
Background offal	mg/kg fw	0.004	MAFF (1995)
Background milk	mg/kg fw	0.002	MAFF (1995)
Background butter	mg/kg fw	0.002	MAFF (1995)
Background eggs	mg/kg fw	0.002	MAFF (1995)
Background outdoor air	mg/m³	1.90×10^{-3}	Calculated from VMM (1999, 2000)
Background indoor air	mg/m³	1.90×10^{-3}	= outdoor air
Background drinking water	mg/m³	3.33×10^{-2}	VMM (2006) – value for xylene divided by 3

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.

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 m³/mol	713 (25°C)	average
log Kow	g/g	3.16	Geometric mean
log Koc	dm³/kg	2.47	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	1.6×10^{-6}	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.6648	average
Diffusion coefficient water (Dw)	m²/d	7.06×10^{-5}	average
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	3.00×10^{-2}	N US-EPA (1995, 2003)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		3 D	IARC (1999a) US-EPA IRIS date not found, before 2002
Systemic effects threshold			
TDI oral	mg/kg.d	1.79×10^{-1}	WHO (1996)
TCL inhalation[a)]	mg/m³	8.7×10^{-1}	WHO (2000)
TDI dermal	mg/kg.d	1.79×10^{-1}	N = oral value
averaging period		child, adolescent, adult	
Limit in air	mg/m³	8.70×10^{-1}	WHO (2000)
Limit value in drinking water	mg/m³	500	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	7.00×10^{-5}	MAFF (1995)

Parameter	Unit	Value	Source
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	Cornelis et al. (2013b)
Background potatoes	mg/kg fw	0.002	MAFF (1995)
Background root crops	mg/kg fw	0.002	MAFF (1995)
Background bulbous plants (onion …)	mg/kg fw	0.002	MAFF (1995)
Background fruit vegetables	mg/kg fw	0.002	MAFF (1995)
Background cabbage	mg/kg fw	0.002	MAFF (1995)
Background leafy vegetables	mg/kg fw	0.002	MAFF (1995)
Background legume	mg/kg fw	0.002	MAFF (1995)
Background beef	mg/kg fw	0.007	MAFF (1995)
Background offal	mg/kg fw	0.004	MAFF (1995)
Background milk	mg/kg fw	0.002	MAFF (1995)
Background butter	mg/kg fw	0.002	MAFF (1995)
Background eggs	mg/kg fw	0.002	MAFF (1995)
Background outdoor air	mg/m³	1.90×10^{-3}	Calculated from VMM (1999, 2000)
Background indoor air	mg/m³	1.90×10^{-3}	= outdoor air
Background drinking water	mg/m³	3.33×10^{-2}	VMM (2006) – value for xylene divided by 3

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.

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 m³/mol	271 (25°C)	average
log Kow	g/g	2.97	Geometric mean
log Koc	dm³/kg	2.86	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	$2x10^{-6}$	van den Berg (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.6144	average
Diffusion coefficient water (Dw)	m²/d	$6.96x10^{-5}$	average
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	$3.00x10^{-2}$	N US-EPA (1995, 2003)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	
BTF kidney	d/kg	calculated	
BTF milk	d/kg	calculated	N
BTF soil – egg	d/kg	0	N values not searched for
BTF feed - egg	d/kg	0	N values not searched for
Carcinogenicity		2B	IARC (2002)
Systemic effects threshold			
TDI oral	mg/kg.d	$7.7x10^{-3}$	WHO (1996)
TCL inhalation[a)]	mg/m³	$2.6x10^{-1}$	WHO (2000)
TDI dermal	mg/kg.d	$7.7x10^{-3}$	N = oral value
averaging period		child, adolescent, lifelong	
Limit in air	mg/m³	$2.60x10^{-1}$	WHO (2000)
Limit value in drinking water	mg/m³	20	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	$5.70x10^{-5}$	MAFF (1999)
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	N Cornelis et al. (2013b)
Background potatoes	mg/kg fw	0.00015	MAFF (1999)

Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0.00015	MAFF (1999)
Background bulbous plants (onion …)	mg/kg fw	0.00015	MAFF (1999)
Background fruit vegetables	mg/kg fw	0.00085	MAFF (1999)
Background cabbage	mg/kg fw	0.00085	MAFF (1999)
Background leafy vegetables	mg/kg fw	0.00045	MAFF (1999)
Background legume	mg/kg fw	0.00085	MAFF (1999)
Background beef	mg/kg fw	0.007	MAFF (1999)
Background offal	mg/kg fw	0.004	MAFF (1999)
Background milk	mg/kg fw	0.002	MAFF (1999)
Background butter	mg/kg fw	0.002	MAFF (1999)
Background eggs	mg/kg fw	0.002	MAFF (1999)
Background outdoor air	mg/m³	4.00×10^{-4}	VMM (1998)
Background indoor air	mg/m³	4.00×10^{-4}	= outdoor air
Background drinking water	mg/m³	1.00×10^{-1}	VMM (2006)

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.

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. (2013a).

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 m³/mol	401 (25°C)	Calculated from S and P
log Kow [a)]	g/g	3.6 (25°C)	Geometric mean
log Koc	dm³/kg	2.836957	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	$6.4x10^{-6}$	van den Berg (1997)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.696 (25°C)	Calculated value
Diffusion coefficient water (Dw)	m²/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 [b)]	mg/m³	$5.83x10^{-3}$	CEHT (2001)
TDI dermal	mg/kg.d	$5x10^{-2}$	N = oral value
averaging period		Child, adolescent, adult	
Limit in air	mg/m³	$5.83x10^{-3}$	CEHT, 2001

Parameter	Unit	Value	Source
Limit value in drinking water	mg/m³	150	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	
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/m³	4.25×10^{-4}	calculated from VMM (1999, 2000)
Background indoor air	mg/m³	4.25×10^{-4}	= outdoor air
Background drinking water	mg/m³	0	

a) The substance data sheet mentions Kow = 3.6. The correct value is log Kow = 3.6. The latter value was used in the calculation of clean-up values and is also used in the Vlier-Humaan model.

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.

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 m³/mol	631 (25°C)	Calculated from S and P
log Kow [a)]	g/g	3.6 (25°C)	Geometric mean
log Koc	dm³/kg	3.106871	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	$6.4x10^{-6}$	van den Berg (1997)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.6864 (25°C)	Calculated value
Diffusion coefficient water (Dw)	m²/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 (non-traceable)
Systemic effects threshold			
TDI oral	mg/kg.d	0.05	CEHT (2001)
TCL inhalation [b)]	mg/m³	$5.83x10^{-3}$	CEHT (2001) and RAIS 2002? /RAIS cannot be traced back
TDI dermal	mg/kg.d	0.05	N = oral value
averaging period		child, adolescent, adult	
Limit in air	mg/m³	$5.83x10^{-3}$	US-EPA, 1997 and RAIS, 2002?, cannot be traced back
Limit value in drinking water	mg/m³	150	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	1.67E-04	?

Parameter	Unit	Value	Source
Dietary background children	mg/kg.day	relative to adult value (cfr. TGD)	↑ Cornelis et al. (2013b)
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/m³	1.53E-03	calculated from VMM (1999, 2000)
Background indoor air	mg/m³	1.53E-03	↑ = outdoor air
Background drinking water	mg/m³	0	↑

a) The substance data sheet mentions Kow = 3.6. The correct value is log Kow = 3.6. The latter value was used in the calculation of clean-up values and is also used in the Vlier-Humaan model.

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.

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 m³/mol	774 (25°C)	Calculated from S and P
log Kow [a)]	g/g	3.7 (25°C)	Geometric mean
log Koc	dm³/kg	2.832509	Geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	6.4E-06	van den Berg (1997)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.6864 (25°C)	calculated value
Diffusion coefficient water (Dw)	m²/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 [b)]	mg/m³	$5.83x10^{-3}$	RAIS (2002) cannot be traced back
TDI dermal	mg/kg.d	0.05	N = oral value
averaging period		child, adolescent, adult	
Limit in air	mg/m³	$5.83x10^{-3}$	RAIS (2002) (cannot be traced back)
Limit value in drinking water	mg/m³	150	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	

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/m³	5.00×10^{-4}	calculated from VMM (1999, 2000)
Background indoor air	mg/m³	5.00×10^{-4}	= outdoor air
Background drinking water	mg/m³	0	

a) The substance data sheet mentions Kow = 3.6. The correct value is log Kow = 3.6. The latter value was used in the calculation of clean-up values and is also used in the Vlier-Humaan model.

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.

REFERENCES

ATSDR. (2007). Toxicological Profile for benzene.

CEHT. (2001). Technical report: development of Cleanup Target Levels (CTLs) for Chapter 62-777.

Cornelis, C., Bierkens, J., & Standaert, A. (2013a). Doorrekening van bodemsaneringsnormen met S-Risk - verkennende oefening.

Cornelis, C., Standaert, A., & Willems, H. (2013b). S-Risk - Technical guidance document.

IARC. (1999a). Re-evaluation of some organic chemicals, Hydrazine and hydrogen Peroxide. *Volume 71*.

IARC. (1999b). Some industrial chemicals and dyestuffs. *Volume 29*.

IARC. (2000). Some industrial chemicals. *Volume 77*.

IARC. (2002). Some traditional herbal medicines, some mycotoxins, naphthalene and styrene. *Volume 82*.

MAFF. (1995). Benzene and other aromatic hydrocarbons in food - average UK dietary intakes.

MAFF. (1999). Total diet study: styrene.

OVAM. (2003a). Aanvulling bij basisinformatie voor risico-evaluaties - polyaromatische koolwaterstoffen en MTBE.

OVAM. (2003b). Aanvulling bij basisinformatie voor risico-evaluaties - trimethylbenzenen.

OVAM. (2004). Basisinformatie voor risico-evaluaties / Deel 4 - SN - Stofdata normering. *Achtergronddocumenten bodemsanering*, 1-78.

OVAM. (2005a). Aanvulling bij basisinformatie voor risico-evaluaties - aangepaste toetsingscriteria voor historische bodemverontreiniging met benzo(a)pyreen en dibenzo(a,h)antraceen.

OVAM. (2005b). Aanvulling bij basisinformatie voor risico-evaluaties - chloorfenolen: voorstel van normering en stofdata.

OVAM. (2009a). Aanvulling bij basisinformatie voor risico-evaluaties - BTEXS stofdata.

OVAM. (2009b). Aanvulling bij basisinformatie voor risico-evaluaties - carcinogene gechloreerde koolwaterstoffen (1,2-DCA, VC, CHL en HCB): stofdata.

OVAM. (2009c). Aanvulling bij basisinformatie voor risico-evaluaties - zware metalen en arseen: stofdata.

OVAM. (2009d). Rekenmodule voor de opname van zware metalen in planten en transfer naar de voedselketen.

Richtlijn 2000/69/EG van het Europees Parlement en de Raad van 16 november 2000 betreffende grenswaarden voor benzeen en koolstofmonoxide in de lucht. (2000). (200/69/EG).

US-EPA. (1991). IRIS - Ethylbenzene (CAS n° 100-41-4).

US-EPA. (1995). Technical Guidance Manual - Assessing dermal contact with soil / existing guidance.

US-EPA. (2000a). IRIS - Benzene (CAS n° 71-43-2).

US-EPA. (2000b). IRIS - Toluene (CAS n° 108-88-3).

US-EPA. (2003). Updated dermal exposure assessment guidance.

US-EPA. (2004). Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment).

van den Berg, R. (1995). Blootstelling van de mens aan bodemverontreiniging. Een kwalitatieve en kwantitatieve analyse, leidend tot voorstellen voor humaan toxicologische C-toetsingswaarden (Herziene versie).

van den Berg, R. (1997). Verantwoording van gegevens en procedures voor de 1e tranche interventiewaarden: van RIVM-rapporten naar de Notitie Interventiewaarden bodemsanering.

VMM. (1998). Luchtkwaliteit in het Vlaamse Gewest.

VMM. (1999). Luchtkwaliteit in het Vlaamse Gewest 1998.

VMM. (2000). Luchtkwaliteit in het Vlaamse Gewest 1999.

VMM. (2006). Deel3: Drinkwaterkwaliteit in detail bekeken. *Kwaliteit van het drinkwater*.

WHO. (1996). Guidelines for drinking-water quality, 2nd Ed. Vol. 2, Health criteria and other supporting information.

WHO. (2000). Air quality guidelines for Europe, 2nd Ed.*, 91*.