Final report

S-Risk Substance Data Sheets – Part 5: Hexane, heptane, octane, MTBE and cyanides

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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 coëfficiënt soil-water
Koa	Distribution coefficient octanol-air
Koc	Distribution coefficient organic carbon-water
Kow	Distribution coefficient octanol-water
Kp	Dermale permeability coefficient
MTBE	methyl-t-butylether
OVAM	Openbare Vlaamse Afvalstoffenmaatschappij (Public Waste Agency of Flanders)
PAH	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)

Hexane, heptane, octane, MTBE and cyanides

LIST OF MODIFICATIONS

12/01/2017   The CAS number of hexane was 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 8.   SUBSTANCE DATA SHEET ALKANES AND MTBE

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. (2013a).

8.1. HEXANE

Parameter	Unit	Value	Source
CAS nr.		110-54-3	ATSDR (1999) – n-hexane
Type		organic	
Dissociating		no	
Molecular weight	g/mol	86	
Solubility	mg/l	9.50 (20°C)	Verschueren (1983)
Vapour pressure	Pa	16000 (20°C)	Verschueren (1983)
Henry-coefficient	Pa m³/mol	calculated	
log Kow	g/g	2.77	Heath et al. (1993)
log Koc	dm³/kg	2.95	Heath et al. (1993)
Log Koa	g/g	calculated	Ⓝ
BCF		calculated	
Dpe	m²/d	4.00×10^{-6}	Van den Berg (1994)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.648	Heath et al. (1993)
Diffusion coefficient water (Dw)	m²/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		Non-carcinogen	No reference
Systemic effects threshold			
TDI oral	mg/kg.d	6×10^{-2}	US-EPA IRIS 1994 (untraceable, outdated)
TCL inhalation[a]	mg/m³	2×10^{-1}	US-EPA IRIS 1995 (untraceable, outdated)
TDI dermal	mg/kg.d	6×10^{-2}	= oral value
Averaging period		child, adolescent, adult	

Parameter	Unit	Value	Source
Limit value in air	mg/m³	2.00×10^{-1}	US-EPA, 1995 (no longer traceable, outdated)
Limit value in drinking water	mg/m³	10	Flemish Government (1989)(maximum level of mineral oil in drinking water)
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	-	
Background food adults	mg/kg day	0	
Background food children	mg/kg.day	0	
Background potato	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	2.20×10^{-3}	VMM (1992)
Background indoor air	mg/m³	2.20×10^{-3}	= outdoor air
Background drinking water	mg/m³	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..

8.2. HEPTANE

Parameter	Unit	Value	Source
CAS nr.		142-82-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	100	
Solubility	mg/l	3 (20°C)	Verschueren (1983)
Vapour pressure	Pa	4700 (20°C)	Verschueren (1983)
Henry-coefficient	Pa m³/mol	calculated	
log Kow	g/g	3.92	Van den Berg (1994)
log Koc	dm³/kg	calculated	
Log Koa	g/g	calculated	Ⓝ
BCF		calculated	
Dpe	m²/d	4.00×10^{-6}	Van den Berg (1994)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.5592	Van den Berg (1994)
Diffusion coefficient water (Dw)	m²/d	calculated	
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		non-carcinogen	?
Systemic effects threshold			
TDI oral	mg/kg.d	3.1	Vermeire et al. (1991)
TCL inhalation[a)]	mg/m³	19	calculated from oral value
TDI dermal	mg/kg.d	3.1	= oral value
Averaging period		child, adolescent, adult	
Limit value in air	mg/m³	19	calculated from oral value
Limit value in drinking water	mg/m³	10	Flemish Government (1989)(maximum level of mineral oil in drinking water)
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	-	
Background food adults	mg/kg day	0	
Background food children	mg/kg.day	0	

Parameter	Unit	Value	Source
Background potato	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	1.00×10^{-3}	VMM (1992)
Background indoor air	mg/m³	1.00×10^{-3}	= outdoor air
Background drinking water	mg/m³	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.

Hexane, heptane, octane, MTBE and cyanides

8.3. OCTANE

Parameter	Unit	Value	Source
CAS nr.		111-65-9	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	114	
Solubility	mg/l	$6.60.10^{-1}$ (20°C)	Verschueren (1983)
Vapour pressure	Pa	1470 (20°C)	Verschueren (1983)
Henry-coefficient	Pa m³/mol	calculated	
log Kow	g/g	4.4	Van den Berg (1994)
log Koc	dm³/kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	3.40×10^{-6}	Van den Berg (1994)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	0.5208	Van den Berg (1994)
Diffusion coefficient water (Dw)	m²/d	calculated	
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		non-carcinogenic	? no reference was given
Systemic effects threshold			
TDI oral	mg/kg.d	3.1	Vermeire et al. (1991)
TCL inhalation[a)]	mg/m³	19	Calculated from oral value
TDI dermal	mg/kg.d	3.1	= oral value
Limit value in air	mg/m³	19	Calculated from oral value
Limit value in drinking water	mg/m³	10	Flemish Government (1989)(maximum level of mineral oil in drinking water)
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	-	
Background food adults	mg/kg day	0	
Background food children	mg/kg.day	0	
Background potato	mg/kg fw	0	

Hexane, heptane, octane, MTBE and cyanides

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/m³	4.00×10^{-4}	VMM (1992)
Background indoor air	mg/m³	4.00×10^{-4}	N = outdoor air
Background drinking water	mg/m³	0	N 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.

Hexane, heptane, octane, MTBE and cyanides

8.4. METHYL-T-BUTYLETHER (MTBE)

Parameter	Unit	Value	Source
CAS nr.		1634-04-4	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	88.15	
Solubility	mg/l	4.20×10^4	Stephenson (1992)
Vapour pressure	Pa	26800	ECB (2000)
Henry-coefficient	Pa m³/mol	43.8	Robbins (1993)
log Kow	g/g	1.14	Average
log Koc	dm³/kg	0.826075	geometric mean
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m²/d	1.00×10^{-7}	Kreule (1995)
Dpvc	m²/d	calculated	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	1.09×10^{-1}	N Fan et al. (2007)
FA	-	1	N
ABS dermal soil/dust	-	0	N negligible
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 (not classifiable)	IARC (1999)
		No classification	US-EPA (1993)
Systemic effects threshold			
TDI oral	mg/kg.d	1.10^{-1}	US-EPA (1997)
TCL inhalation[a)]	mg/m³	3	US-EPA (1993)
TDI dermal	mg/kg.d	1.10^{-1}	= oral value
Averaging period		child, adolescent, adult	
Limit value in air	mg/m³	3	US-EPA (1993)
Limit value in drinking water	mg/m³	300	Calculated from oral 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	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Background food adults	mg/kg day	0	
Background food children	mg/kg.day	0	
Background potato	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/m³	1.00×10^{-3}	No reference in substance data sheet
Background indoor air	mg/m³	1.00×10^{-3}	N = outdoor air
Background drinking water	mg/m³	1.00×10^{-1}	N

[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 9.   SUBSTANCE DATA SHEETS CYANIDES

Indien stoffengegevens niet overgenomen zijn uit de stoffenfiches, wordt dit aangeduid met $\boxed{N}$ en eventueel een toelichting. Gedetailleerde informatie voor nieuwe gegevens is opgenomen in Cornelis et al. (2013a).

9.1. FREE CYANIDE

Parameter	Unit	Value	Source
CAS nr.		57-12-5	
Type		organic	
Dissociating			
Acid dissociation[)]		Considered non-dissociating	$\boxed{N}$
(pKa		9.2	$\boxed{N}$ not used)
Molecular weight	g/mol	26	(expressed as CN-)
Solubility	mg/l	1.00×10^6	miscible (arbitrarily high value)
Vapour pressure	Pa	83993 (20°C) (HCN)	ATSDR (1997)
Henry-coefficient	Pa m³/mol	5168 (20°C)	ATSDR (1997)
log Kow	g/g	0.87	ATSDR (1997)
log Koc	dm³/kg	3 (KCN)	ATSDR (1997)
Log Koa	g/g	calculated	$\boxed{N}$
BCF		0	Towill et al. (1978)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	5.50×10^{-4}	$\boxed{N}$ average of Dugard (1987) in Johanson (2008)
FA	-	1	$\boxed{N}$
ABS dermal soil/dust	-	1.00×10^{-1}	$\boxed{N}$ Cal-EPA (1999)
BTF beef	d/kg	0	
BTF mutton	d/kg	0	$\boxed{N}$
BTF liver	d/kg	0	$\boxed{N}$
BTF kidney	d/kg	0	$\boxed{N}$
BTF milk	d/kg	0	
BTF soil – egg	d/kg	0	$\boxed{N}$ values not searched for
BTF feed - egg	d/kg	0	$\boxed{N}$ values not searched for
Carcinogenicity		D niet klasseerbaar als menselijk carcinigeen	US-EPA IRIS, 1998 (untraceable, outdated)
Systemic effects threshold			
TDI oral	mg/kg.d	1.2×10^{-2}	WHO (1996)
TCL inhalation[a)]	mg/m³	2×10^{-1}	Vermeire (1991)

Parameter	Unit	Value	Source
TDI dermal	mg/kg.d	$1.2x10^{-2}$	= oral value
Limit value in air	mg/m³	$2.00x10^{-1}$	Vermeire (1991)
Limit value in drinking water	mg/m³	70	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	-	
Background food adults	mg/kg day	0	Vermeire (1991)
Background food children	mg/kg.day	0	
Background potato	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	0	
Background indoor air	mg/m³	0	= outdoor air
Background drinking water	mg/m³	0	

[a] In case of an acid dissiociating chemical, Vlier-Humaan calculated the Kd from the Koc (the Koc value for free cyanide in the substance data sheet = 1000 (value for KCN)). S-Risk calculates the Kd for dissociating chemicals directly from the Koc. Because of the impact this has on the results, free cyanide has been entered in S-Risk as a nondissociating chemical to enable the use of the Koc. The influence of the pH on the calculated risks is not visible in the pH range of < 7.5 and very small at pH = 8.

[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.

9.2. NON-CHLORO OXIDIZABLE CYANIDES (COMPLEX CYANIDES)

Parameter	Unit	Value	Source
CAS nr.		-	
Type		anorganic	
Molecular weight	g/mol	26	(expressed as CN-)
Solubility	mg/l	26	Meeussen (1992)
Vapour pressure	Pa	0	
Henry-coefficient	Pa m³/mol	0	
Kd	dm³/kg	0	
BCF		2.82 for root vegetables 1.41 for aboveground vegetables	calculated from Wallace et al. (1977)
Dpe	m²/d	0	
Dpvc	m²/d	0	
Diffusion coefficient air (Da)	m²/d	calculated	
Diffusion coefficient water (Dw)	m²/d	calculated	
Kp	[cm/h]	0	🔃
FA	-	1	🔃
ABS dermal soil/dust	-	1.00×10^{-2}	🔃 Cal-EPA (1999)
BTF beef	d/kg	0	
BTF mutton	d/kg	0	🔃
BTF liver	d/kg	0	🔃
BTF kidney	d/kg	0	🔃
BTF milk	d/kg	0	
BTF soil – egg	d/kg	0	🔃 values not searched for
BTF feed - egg	d/kg	0	🔃 values not searched for
Carcinogenicity		non-carcinogenic	? no reference
Systemic effects threshold			
TDI oral	mg/kg.d	1.3×10^{-2}	Vermeire et al. (1991)
TCL inhalation[a)]	mg/m³	1	ACROS (1998)
TDI dermal	mg/kg.d	1.3×10^{-2}	= oral value
Averaging period		child, adolescent, adult	
Limit value in air	mg/m³	1	ACROS (1998)
Limit value in drinking water	mg/m³	70	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	-	
Background food adults	mg/kg day	4.00×10^{-4}	Vermeire et al. (1991)
Background food children	mg/kg.day	relative to adult value (cfr. TGD)	🔃 Cornelis et al. (2013b)
Background potato	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/m³	0	
Background indoor air	mg/m³	0	$\mathbb{N}$ = outdoor air
Background drinking water	mg/m³	0	$\mathbb{N}$

[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.

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