

Final report

# S-Risk for the Walloon region - 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
ISSeP	Institut Scientifique de Service Public
K <sub>d</sub>	Sorption coefficient 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

## INTRODUCTION

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

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

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

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

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

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

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

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

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

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

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

The substance data sheets consist of 6 documents:

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

**Hexane, heptane, octane, MTBE and cyanides**

- 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 8. SUBSTANCE DATA SHEET ALKANES AND MTBE

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.

## 8.1. HEXANE

Parameter	Unit	Value	Source
CAS nr.		110-54-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	86	
Solubility	mg/l	9.50 (20°C)	Verschuere (1983)
Vapour pressure*	Pa	16000 (20°C)	Verschuere (1983)
Henry-coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	2.77	Heath et al. (1993)
log Koc	dm <sup>3</sup> /kg	2.95	Heath et al. (1993)
Log Koa	g/g	calculated	<b>N</b>
BCF		calculated	
Dpe	m <sup>2</sup> /d	4.00x10 <sup>-6</sup>	Van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.648	Heath et al. (1993)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	<b>N</b>
FA	-	1	<b>N</b>
ABS dermal soil/dust	-	0	<b>N</b> negligible, volatile chemical
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	<b>N</b>
BTF liver	d/kg	calculated	<b>N</b>
BTF kidney	d/kg	calculated	<b>N</b>
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	<b>N</b> values not searched for
BTF feed - egg	d/kg	0	<b>N</b> values not searched for
Carcinogenicity		D	<b>W</b> US-EPA (2005)
Systemic effects threshold			
TDI oral	mg/kg.d	1.0x10 <sup>-1</sup>	<b>W</b> Health Canada (2004)
TCL inhalation	mg/m <sup>3</sup>	2.0x10 <sup>-1</sup>	<b>W</b> US-EPA (1990)
TDI dermal	mg/kg.d	1.0x10 <sup>-1</sup>	= oral value
Averaging period		child, adolescent, adult	
Limit value in outdoor air	mg/m <sup>3</sup>	-	<b>W</b>

Hexane, heptane, octane, MTBE and cyanides



Parameter	Unit	Value	Source
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
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/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

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

## 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 m <sup>3</sup> /mol	calculated	
log Kow	g/g	3.92	Van den Berg (1994)
log Koc	dm <sup>3</sup> /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	4.00x10 <sup>-6</sup>	Van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.5592	Van den Berg (1994)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	3.00x10 <sup>-2</sup>	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		D	W US-EPA (1996)
Systemic effects threshold			
TDI oral	mg/kg.d	3.1	Vermeire et al. (1991)
TCL inhalation	mg/m <sup>3</sup>	0.35	W TX (2012)
TDI dermal	mg/kg.d	3.1	= oral value
Averaging period child, adolescent, adult			
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
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/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	

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

## 8.3. OCTANE

Parameter	Unit	Value	Source
CAS nr.		111-65-9	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	114	
Solubility	mg/l	$6.60 \cdot 10^{-1}$ (20°C)	Verschueren (1983)
Vapour pressure*	Pa	1470 (20°C)	Verschueren (1983)
Henry-coefficient	Pa m <sup>3</sup> /mol	calculated	
log Kow	g/g	4.4	Van den Berg (1994)
log Koc	dm <sup>3</sup> /kg	calculated	
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m <sup>2</sup> /d	$3.40 \cdot 10^{-6}$	Van den Berg (1994)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	0.5208	Van den Berg (1994)
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	$3.00 \cdot 10^{-2}$	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		not classified	no reference
Systemic effects threshold			
TDI oral	mg/kg.d	3.1	Vermeire et al. (1991)
TCL inhalation	mg/m <sup>3</sup>	0.35	W TX (2003)
TDI dermal	mg/kg.d	3.1	= oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	-	W
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
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	

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

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

## 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	4.20x10 <sup>4</sup>	Stephenson (1992)
Vapour pressure*	Pa	26800	ECB (2000)
Henry-coefficient	Pa m <sup>3</sup> /mol	43.8	Robbins (1993)
log Kow	g/g	1.14	Average
log Koc	dm <sup>3</sup> /kg	0.826075	geometric mean
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m <sup>2</sup> /d	1.00x10 <sup>-7</sup>	Kreule (1995)
Dpvc	m <sup>2</sup> /d	calculated	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	1.09x10 <sup>-1</sup>	Fan et al. (2007)
FA	-	1	
ABS dermal soil/dust	-	0	negligible
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	
BTF liver	d/kg	calculated	
BTF kidney	d/kg	calculated	
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0	values not searched for
BTF feed - egg	d/kg	0	values not searched for
Carcinogenicity		3	IARC (1999)
Systemic effects threshold			
TDI oral	mg/kg.d	1.10 <sup>-2</sup>	Health Canada (1996)
TCL inhalation	mg/m <sup>3</sup>	3.0	US-EPA (1993)
TDI dermal	mg/kg.d	1.10 <sup>-2</sup>	= oral value
Averaging period child, adolescent, adult			
Systemic effects non-threshold			
Oral slope factor	(mg/kg.d) <sup>-1</sup>	1.0x10 <sup>-8</sup>	dummy value (considered non-carcinogenic by oral exposure)
Inhalation unit risk	(mg/m <sup>3</sup> ) <sup>-1</sup>	2.6x10 <sup>-4</sup>	OEHHA (1999)
Dermal slope factor	(mg/kg.d) <sup>-1</sup>	1.0x10 <sup>-8</sup>	= oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	
Limit value in drinking water	mg/m <sup>3</sup>	-	
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	

Parameter	Unit	Value	Source
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/m <sup>3</sup>	0	W
Background indoor air	mg/m <sup>3</sup>	0	W
Background drinking water	mg/m <sup>3</sup>	0	W

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

## CHAPTER 9. SUBSTANCE DATA SHEETS CYANIDES

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.

## 9.1. FREE CYANIDE

Parameter	Unit	Value	Source
CAS nr.		57-12-5	
Type		organic	
Dissociating			
Acid dissociation		Considered non-dissociating	<b>N</b>
pKa		9.2	<b>N</b> not used)
Molecular weight	g/mol	26	(expressed as CN-)
Solubility	mg/l	1.00x10 <sup>6</sup>	miscible (arbitrarily high value)
Vapour pressure*	Pa	83993 (20°C) (HCN)	ATSDR (1997)
Henry-coefficient	Pa m <sup>3</sup> /mol	5168 (20°C)	ATSDR (1997)
log Kow	g/g	0.87	ATSDR (1997)
log Koc	dm <sup>3</sup> /kg	3 (KCN)	ATSDR (1997)
Log Koa	g/g	calculated	<b>N</b>
BCF		0	Towill et al. (1978)
Dpe	m <sup>2</sup> /d	0	
Dpvc	m <sup>2</sup> /d	0	
Diffusion coefficient air (Da)	m <sup>2</sup> /d	calculated	
Diffusion coefficient water (Dw)	m <sup>2</sup> /d	calculated	
Kp	[cm/h]	5.50x10 <sup>-4</sup>	<b>N</b> average of Dugard (1987) in Johanson (2008)
FA	-	1	<b>N</b>
ABS dermal soil/dust	-	1.00x10 <sup>-1</sup>	<b>N</b> Cal-EPA (1999)
BTF beef	d/kg	0	
BTF mutton	d/kg	0	<b>N</b>
BTF liver	d/kg	0	<b>N</b>
BTF kidney	d/kg	0	<b>N</b>
BTF milk	d/kg	0	
BTF soil – egg	d/kg	0	<b>N</b> values not searched for
BTF feed - egg	d/kg	0	<b>N</b> values not searched for
Carcinogenicity		D	US-EPA (1991)
Systemic effects threshold			
TDI oral	mg/kg.d	1.2x10 <sup>-2</sup>	WHO (1996)
TCL inhalation	mg/m <sup>3</sup>	3.0x10 <sup>-3</sup>	<b>W</b> US-EPA (1994)



Parameter	Unit	Value	Source
TDI dermal	mg/kg.d	$1.2 \times 10^{-2}$	= oral value
Limit value in outdoor air	mg/m <sup>3</sup>	-	W
Limit value in drinking water	mg/m <sup>3</sup>	50	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	-	
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/m <sup>3</sup>	0	
Background indoor air	mg/m <sup>3</sup>	0	
Background drinking water	mg/m <sup>3</sup>	0	

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

a) In case of an acid dissociating 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.

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