

Final report

S-Risk Substance Data Sheets – Part 6: Total Petroleum Hydrocarbons

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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	Dermale permeability coefficient
MTBE	methyl-t-butylether
OVAM	Openbare Vlaamse Afvalstoffenmaatschappij (Public Waste Agency of Flanders)
PAH	polycyclic aromatic hydrocarbons
Ptot	Total phosphorus content
TCA	Tolerable Concentration in Air
TDI	Tolerable Daily Intake
TGD	Technical Guidance Document
VMM	Vlaamse MilieuMaatschappij (Flanders Environment Agency)

LIST OF MODIFICATIONS

- 16/10/2014 The values found at log K_{ow} and log K_{ow} were incorrectly displayed as 10x, the 10 was left out
- 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 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 for benzo(a)pyrene and dibenz(a,h)anthracene;
- Cyanides: OVAM (2004);
- Trimethylbenzenes: OVAM (2003b);
- Chlorophenols: OVAM (2005b)
- Hexane, heptane, octane: OVAM (2004);
- MTBE: OVAM (2003a)

Details on the new information is always available in the report discussing the calculation of clean-up values with S-Risk (Cornelis, Bierkens, 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 polycyclic aromatic hydrocarbons
- Part 5: Substance data sheets alkanes, MTBE and cyanides
- **Part 6: Substance data sheets total petroleum hydrocarbons**

CHAPTER 10. SUBSTANCE DATA SHEET TOTAL PETROLEUM HYDROCARBONS

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).

10.1. ALIPHATIC FRACTION EC 5 – 6


Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	81	TPHCWG (1999)
Solubility	mg/l	3.60×10^1	TPHCWG (1999)
Vapour pressure	Pa	35463 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	80388 (20°C)	TPHCWG (1999)
log Kow	g/g	3.52	Franken et al. (1999)
log Koc	dm ³ /kg	2.9	TPHCWG (1999)
Log Koa	g/g	calculated	
BCF		calculated	
Dpe	m ² /d	4×10^{-6}	Van den Berg et al. (1994) (hexane)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64×10^{-5}	TPHCWG (1999)
Kp	cm/h	calculated	
FA	-	1	
ABS dermal soil/dust	-	0.00	 US-EPA (2003), volatility comparable with benzene
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	0.00	 values not searched for
BTF feed - egg	d/kg	0.00	 values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	2	TPHCWG (1999)
TCA inhalation ^{a)}	mg/m ³	18.4	TPHCWG (1999)
TDI dermal	mg/kg.d	2	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.84×10^1	TPHCWG (1999)

Parameter	Unit	Value	Source
Limit value in drinking water	mg/m ³	6000	calculated on the basis of the TDI
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0.00	
Dietary background children	mg/kg.day	0.00	
Background potatoes	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	8.00x10 ⁻⁴	VMM (1999) (hexane)
Background indoor air	mg/m ³	8.00x10 ⁻⁴	 = outdoor air
Background drinking water	mg/m ³	0.00	 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.

10.2. ALIPHATIC FRACTION EC >6 – 8

Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	100	TPHCWG (1999)
Solubility	mg/l	5.40	TPHCWG (1999)
Vapour pressure	Pa	6383 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	121800 (20°C)	TPHCWG (1999)
log Kow	g/g	3.6	Franken et al. (1999)
log Koc	dm ³ /kg	3.6	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	4.00x10 ⁻⁶	Van den Berg et al. (1994) (heptane)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0,864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	3.00x10 ⁻²	N US-EPA (2003), volatility comparable with toluene, ethylbenzene, xylene
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	2	TPHCWG (1999)
TCA inhalation ^{a)}	mg/m ³	18.4	TPHCWG (1999)
TDI dermal	mg/kg.d	2	= oral value
averaging period		child, adolescent, adult	averaging period
Limit value in air	mg/m ³	1.84x10 ¹	TPHCWG (1999)
Limit value in drinking water	mg/m ³	5400	calculated based on the TDI, adjusted to the solubility limit
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	

Parameter	Unit	Value	Source
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0.00	
Dietary background children	mg/kg.day	0.00	
Background potatoes	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	4.00x10 ⁻⁴	VMM (1999) (octane)
Background indoor air	mg/m ³	4.00x10 ⁻⁴	 = outdoor air
Background drinking water	mg/m ³	0.00	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.

10.3. ALIPHATIC FRACTION EC >8 – 10

Parameter	Unit	Value	Source
CAS nr.			
Type		Organic	
Dissociating		no	
Molecular weight	g/mol	130	TPHCWG (1999)
Solubility	mg/l	4.30×10^{-1}	TPHCWG (1999)
Vapour pressure	Pa	638.3 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	194880 (20°C)	TPHCWG (1999)
log Kow	g/g	3.69	Franken et al. (1999)
log Koc	dm ³ /kg	4.50	TPHCWG (1999)
Log Koa	g/g	calculated	
BCF		calculated	N
Dpe	m ² /d	6.00×10^{-8}	Veenendaal et al. (1985) (nonane)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64×10^{-5}	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.0×10^{-1}	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.1	TPHCWG (1999)
TCA inhalation ^{a)}	mg/m ³	1	TPHCWG (1999)
TDI dermal	mg/kg.d	0.1	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.00	TPHCWG (1999)
Limit value in drinking water	mg/m ³	300	calculated based on the TDI
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	0,00	
Dietary background children	mg/kg.day	0.00	
Background potatoes	mg/kg fw	0.00	

Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	3.30x10 ⁻⁴	VMM (1999) (nonane, type III)
Background indoor air	mg/m ³	3.30x10 ⁻⁴	<input type="checkbox"/> = outdoor air
Background drinking water	mg/m ³	0.00	<input type="checkbox"/> no values

- a) The original substance data sheets express the reference value for inhalation in units of mg/kg.d. S-Risk uses a reference value in units of mg/m³. Conversion can be done by multiplying the value in mg/kg.d with a body weight of 70 kg and an inhalation rate of 20 m³/d.

10.4. ALIPHATIC FRACTION EC >10 – 12

Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		neen	
Molecular weight	g/mol	160	TPHCWG (1999)
Solubility	mg/l	3.40×10^{-2}	TPHCWG (1999)
Vapour pressure	Pa	63.83 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	292320 (20°C)	TPHCWG (1999)
log Kow	g/g	3.76	Franken et al. (1999)
log Koc	dm ³ /kg	5.40	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	6.00×10^{-8}	Veenendaal et al. (1985) (nonane)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64×10^{-5}	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00×10^{-1}	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.1	TPHCWG (1999)
TCA inhalation ^{a)}	mg/m ³	1	TPHCWG (1999)
TDI dermal	mg/kg.d	0.1	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.00	TPHCWG (1999)
Limit value in drinking water	mg/m ³	34	calculated based on the TDI, adjusted to the solubility limit
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	0.00	
Dietary background children	mg/kg.day	0.00	

Parameter	Unit	Value	Source
Background potatoes	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	no values
Background indoor air	mg/m ³	0.00	<input checked="" type="checkbox"/> = outdoor air
Background drinking water	mg/m ³	0.00	<input checked="" type="checkbox"/> no values

- a) The original substance data sheets express the reference value for inhalation in units of mg/kg.d. S-Risk uses a reference value in units of mg/m³. Conversion can be done by multiplying the value in mg/kg.d with a body weight of 70 kg and an inhalation rate of 20 m³/d.

10.5. ALIPHATIC FRACTION EC >12 – 16



Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		neen	
Molecular weight	g/mol	200	TPHCWG (1999)
Solubility	mg/l	7.60x10 ⁻⁴	TPHCWG (1999)
Vapour pressure	Pa	4.86 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	1 266 721 (20°C)	TPHCWG (1999)
log Kow	g/g	3.85	Franken et al. (1999)
log Koc	dm ³ /kg	6.70	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	6.00x10 ⁻⁸	Veenendaal et al. (1985) (nonane)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00x10 ⁻¹	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.1	TPHCWG (1999)
TCA inhalation ^{a)}	mg/m ³	1	TPHCWG (1999)
TDI dermal	mg/kg.d	0.1	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.00	TPHCWG (1999)
Limit value in drinking water	mg/m ³	0.76	calculated based on the TDI, adjusted to the solubility limit
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	0.00	
Dietary background children	mg/kg.day	0.00	

Parameter	Unit	Value	Source
Background potatoes	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	
Background indoor air	mg/m ³	0.00	<input type="checkbox"/> = outdoor air
Background drinking water	mg/m ³	0.00	<input type="checkbox"/> No values

- a) The original substance data sheets express the reference value for inhalation in units of mg/kg.d. S-Risk uses a reference value in units of mg/m³. Conversion can be done by multiplying the value in mg/kg.d with a body weight of 70 kg and an inhalation rate of 20 m³/d.

10.6. ALIPHATIC FRACTION EC >16 – 21



Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	270	TPHCWG (1999)
Solubility	mg/l	2.50x10 ⁻⁶	TPHCWG (1999)
Vapour pressure	Pa	0.111 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	11 936 409 (20°C)	TPHCWG (1999)
log Kow	g/g	3.97	Franken et al. (1999)
log Koc	dm ³ /kg	8.80	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	6.00x10 ⁻⁸	Veenendaal et al. (1985) (nonane)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00x10 ⁻¹	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	2	TPHCWG (1999)
TCA inhalation ^{c)}	mg/m ³	7	calculated based on the TDI
TDI dermal	mg/kg.d	2	= oral value
Limit value in air	mg/m ³	-	TPHCWG (1999)
Limit value in drinking water	mg/m ³	2.50x10 ⁻³	calculated based on the TDI, adjusted to the solubility limit
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	0.00	
Background food children	mg/kg.day	0.00	
Background potato	mg/kg fw	0.00	

Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	
Background indoor air	mg/m ³	0.00	 = outdoor air
Background drinking water	mg/m ³	0.00	 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.

10.7. AROMATIC FRACTION EC 8 – 10



Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	120	TPHCWG (1999)
Solubility	mg/l	6.50x10 ¹	TPHCWG (1999)
Vapour pressure	Pa	638 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	1169 (20°C)	TPHCWG (1999)
log Kow	g/g	3.55	Franken et al. (1999)
log Koc	dm ³ /kg	3.20	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.10x10 ⁻⁶	Van den Berg et al. (1994) (ethylbenzene)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	3.00x10 ⁻²	N US-EPA (2003) volatility comparable with toluene, ethylbenzene, xylene
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	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.04	TPHCWG (1999)
TCA inhalation ^{c)}	mg/m ³	0.2	TPHCWG (1999)
TDI dermal	mg/kg.d	0.04	= oral value
averaging period		Child, adolescent, adult	
Limit value in air	mg/m ³	0.2	TPHCWG (1999)
Limit value in drinking water	mg/m ³	120	calculated based on the TDI
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Background food adults	mg/kg day	0.00	

Parameter	Unit	Value	Source
Background food children	mg/kg.day	0.00	
Background potato	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	1.0x10 ⁻³	VMM (1999), ethylbenzene
Background indoor air	mg/m ³	1.0x10 ⁻³	 = outdoor air
Background drinking water	mg/m ³	0.00	 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.

10.8. AROMATIC FRACTION EC >10 – 12



Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	130	TPHCWG (1999)
Solubility	mg/l	2.50x10 ¹	TPHCWG (1999)
Vapour pressure	Pa	63.8 at (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	341 (20°C)	TPHCWG (1999)
log Kow	g/g	3.58	Franken et al. (1999)
log Koc	dm ³ /kg	3.40	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.10x10 ⁻⁶	Van den Berg et al. (1994) (ethylbenzene)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00x10 ⁻¹	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.04	TPHCWG (1999)
TCA inhalation ^{c)}	mg/m ³	0.2	TPHCWG (1999)
TDI dermal	mg/kg.d	0.04	= oral value
averaging period		Child, adolescent, adult	
Limit value in air	mg/m ³	2.00x10 ⁻¹	TPHCWG (1999)
Limit value in drinking water	mg/m ³	120	calculated based on the TDI
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Background food adults	mg/kg day	0.00	
Background food children	mg/kg.day	0.00	
Background potato	mg/kg fw	0.00	

Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	
Background indoor air	mg/m ³	0.00	 = outdoor air
Background drinking water	mg/m ³	0.00	 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.

10.9. AROMATIC FRACTION EC >12 – 16

Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	150	TPHCWG (1999)
Solubility	mg/l	5.80	TPHCWG (1999)
Vapour pressure	Pa	4.86 (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	129 (20°C)	TPHCWG (1999)
log Kow	g/g	3.61	Franken et al. (1999)
log Koc	dm ³ /kg	3.70	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.10x10 ⁻⁶	Van den Berg et al. (1994) (ethylbenzene)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64x10 ⁻⁵	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00x10 ⁻¹	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.04	TPHCWG (1999)
TCA inhalation ^{c)}	mg/m ³	0.2	TPHCWG (1999)
TDI dermal	mg/kg.d	0.04	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	2.00x10 ⁻¹	TPHCWG (1999)
Limit value in drinking water	mg/m ³	120	calculated based on the TDI
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Background food adults	mg/kg day	0.00	
Background food children	mg/kg.day	0.00	
Background potato	mg/kg fw	0.00	

Parameter	Unit	Value	Source
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	
Background indoor air	mg/m ³	0.00	 = outdoor air
Background drinking water	mg/m ³	0.00	 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.

10.10.AROMATIC FRACTION EC >16 - 21

Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	190	TPHCWG (1999)
Solubility	mg/l	6.5×10^{-1}	TPHCWG (1999)
Vapour pressure	Pa	1.11×10^{-1} (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	3.16×10^1 (20°C)	TPHCWG (1999)
log Kow	g/g	3.66	Franken et al. (1999)
log Koc	dm ³ /kg	4.2	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.00×10^{-7}	Van den Berg et al. (1994) (pyreen)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64×10^{-5}	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00×10^{-1}	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.03	TPHCWG (1999)
TCA inhalation ^{c)}	mg/m ³	0.105	calculated based on the TDI
TDI dermal	mg/kg.d	0.03	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	-	
Limit value in drinking water	mg/m ³	90	calculated based on the TDI
Limit value in plants	mg/kg fw	-	
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	
Milk	mg/kg fw	-	
Butter	mg/kg fw	-	
Egg	mg/kg fw	-	
Background food adults	mg/kg day	2.30×10^{-5}	Vermeire (1993)
Background food children	mg/kg.day	relative to adult value (cfr. TGD)	N Cornelis et al. (2013b)

Parameter	Unit	Value	Source
Background potato	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	
Background indoor air	mg/m ³	0.00	<input checked="" type="checkbox"/> = indoor air
Background drinking water	mg/m ³	0.00	<input checked="" type="checkbox"/> No values

- a) The original substance data sheets express the reference value for inhalation in units of mg/kg.d. S-Risk uses a reference value in units of mg/m³. Conversion can be done by multiplying the value in mg/kg.d with a body weight of 70 kg and an inhalation rate of 20 m³/d.

10.11.AROMATIC FRACTION EC > 21 – 35

Parameter	Unit	Value	Source
CAS nr.		-	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	240	TPHCWG (1999)
Solubility	mg/l	6.60×10^{-3}	TPHCWG (1999)
Vapour pressure	Pa	4.458×10^{-5} (20°C)	TPHCWG (1999)
Henry coefficient	Pa m ³ /mol	1.6321 (20°C)	TPHCWG (1999)
log Kow	g/g	3.74	Franken et al. (1999)
log Koc	dm ³ /kg	5.1	TPHCWG (1999)
Log Koa	g/g	calculated	N
BCF		calculated	
Dpe	m ² /d	2.00×10^{-7}	Van den Berg et al. (1994) (pyrene)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.864	TPHCWG (1999)
Diffusion coefficient water (Dw)	m ² /d	8.64×10^{-5}	TPHCWG (1999)
Kp	cm/h	calculated	N
FA	-	1	N
ABS dermal soil/dust	-	1.00×10^{-1}	N US-EPA (2004)
BTF beef	d/kg	calculated	
BTF mutton	d/kg	calculated	N
BTF liver	d/kg	calculated	N
BTF kidney	d/kg	calculated	N
BTF milk	d/kg	calculated	
BTF soil – egg	d/kg	0.0	N values not searched for
BTF feed - egg	d/kg	0.0	N values not searched for
Carcinogenicity		non-carcinogenic	
Systemic effects threshold			
TDI oral	mg/kg.d	0.03	TPHCWG (1999)
TCA inhalation ^{c)}	mg/m ³	0.105	calculated based on the TDI
TDI dermal	mg/kg.d	0.03	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	-	
Limit value in drinking water	mg/m ³	6.6	calculated based on the TDI, adjusted to the solubility limit
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	2.30×10^{-5}	Vermeire (1993)

Parameter	Unit	Value	Source
Background food children	mg/kg.day	relative to adult value (cfr. TGD)	☒
Background potato	mg/kg fw	0.00	
Background root crops	mg/kg fw	0.00	
Background bulbous plants (onion ...)	mg/kg fw	0.00	
Background fruit vegetables	mg/kg fw	0.00	
Background cabbage	mg/kg fw	0.00	
Background leafy vegetables	mg/kg fw	0.00	
Background legume	mg/kg fw	0.00	
Background beef	mg/kg fw	0.00	
Background offal	mg/kg fw	0.00	
Background milk	mg/kg fw	0.00	
Background butter	mg/kg fw	0.00	
Background eggs	mg/kg fw	0.00	
Background outdoor air	mg/m ³	0.00	
Background indoor air	mg/m ³	0.00	☒ = outdoor air
Background drinking water	mg/m ³	0.00	☒ 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.

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