

Final report

S-Risk Substance Data Sheets – Part 4: Polycyclic Aromatic Hydrocarbons (PAHs)

C. Cornelis, J. Bierkens, A. Standaert

Study accomplished under the authority of OVAM
2016/MRG/R/0513

February 2017



VITO NV

Boeretang 200 - 2400 MOL - BELGIE

Tel. + 32 14 33 55 11 - Fax + 32 14 33 55 99

vito@vito.be - www.vito.be

BTW BE-0244.195.916 RPR (Turnhout)

Bank 375-1117354-90 ING

BE34 3751 1173 5490 - BBRUBEBB

All rights, amongst which the copyright, on the materials described in this document rest with the Flemish Institute for Technological Research NV ("VITO"), Boeretang 200, BE-2400 Mol, Register of Legal Entities VAT BE 0244.195.916.

The information provided in this document is confidential information of VITO. This document may not be reproduced or brought into circulation without the prior written consent of VITO. Without prior permission in writing from VITO this document may not be used, in whole or in part, for the lodging of claims, for conducting proceedings, for publicity and/or for the benefit or acquisition in a more general sense.

TABLE OF CONTENTS

Table of Contents	I
List of Acronyms	II
List of modifications	III
Introduction	5
CHAPTER 7. Substance Data Sheets polycyclic aromatic hydrocarbons	7
7.1. <i>Acenaphthene</i>	7
7.2. <i>Acenaphthylene</i>	10
7.3. <i>Anthracene</i>	12
7.4. <i>Benzo(a)anthracene</i>	14
7.5. <i>Benzo(a)pyrene</i>	16
7.6. <i>Benzo(b)fluoranthene</i>	18
7.7. <i>Benzo(g,h,i)perylene</i>	20
7.8. <i>Benzo(k)fluoranthene</i>	22
7.9. <i>Chrysene</i>	24
7.10. <i>Dibenz(a,h)anthracene</i>	26
7.11. <i>Fenanthrene</i>	28
7.12. <i>Fluoranthene</i>	30
7.13. <i>Fluorene</i>	32
7.14. <i>Indeno(1,2,3-cd)pyrene</i>	34
7.15. <i>Naphthalene</i>	36
7.16. <i>Pyrene</i>	38
References	40

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
K _{oa}	Distribution coefficient octanol-air
K _{oc}	Distribution coefficient organic carbon-water
K _{ow}	Distribution coefficient octanol-water
K _p	Dermale permeability coefficient
MTBE	methyl-t-butylether
OVAM	Openbare Vlaamse Afvalstoffenmaatschappij (Public Waste Agency of Flanders)
PAH	polycyclic aromatic hydrocarbons
P _{tot}	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

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 7. SUBSTANCE DATA SHEETS POLYCYCLIC AROMATIC 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).

7.1. ACENAPHTHENE

Parameter	Unit	Value	Source
CAS nr.		83-32-9	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	154	Verschueren (1983)
Solubility	mg/l	3.93 (25°C)	WHO (1998)
Vapour pressure	Pa	0.29 (25°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	14.8 (25°C)	WHO (1998)
log Kow	g/g	3.92	WHO (1998)
log Koc	dm ³ /kg	4.25	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	 ^{a)}
Dpe	m ² /d	5.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	 US-EPA (2004)
ABS dermal soil/dust	-	1.30x10 ⁻¹	 US-EPA (2004)
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	 Low recovery in egg yolk in investigated PAHs (Fournier, Feidt, Dziurla, Grandclaudon, and Jondreville, 2010)
BTF feed - egg	d/kg	0	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		not evaluated D	IARC (1998) Baars et al. (2001)
Systemic effects threshold			 Not included in calculation of soil remediation value
TDI oral	mg/kg.d	6x10 ⁻²	US-EPA (1991)

Parameter	Unit	Value	Source
TCA inhalation ^{a)}	mg/m ³	2.1x10 ⁻¹	Nouwen et al. (2000)
TDI dermal	mg/kg.d	6x10 ⁻²	= oral value
averaging period		child, adolescent, adult	
Systemic effects no threshold ^{d)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6x10 ⁻⁴	Carcinogenic potency= 0.001 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7x10 ⁻²	Carcinogenic potency = 0.001 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6x10 ⁻⁴	= oral value
Limit value in air	mg/m ³	1.20x10 ⁻⁴	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	180	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	-	
Dietary background adults	mg/kg day	1.40x10 ⁻⁵	 SCF (2002) in Nouwen et al. (2000)
Dietary background children	mg/kg.day	relative to adults (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/m ³	0	
Background indoor air	mg/m ³	0	 = outdoor air
Background drinking water	mg/m ³	0	



- a) For the calculation of soil remediation values, BCF values were filled in (BCF aboveground plant parts and root vegetables set at 2.32 mg/kg dm per mg/kg dm)
- b) Acenaphthene has been considered a nonthreshold carcinogen when calculating the soil remediation values. The background report also provides values for non-carcinogenic effects. These were taken up in the S-Risk substance data sheet.
- c) 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.

Polycyclic Aromatic Hydrocarbons (PAHs)

- d) 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1 \cdot 10^{-5} / (\text{dose at } 1 \cdot 10^{-5} \text{ (mg}/\text{kg}\cdot\text{d}))$. 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).

7.2. ACENAPHTHYLENE

Parameter	Unit	Value	Source
CAS nr.		208-96-8	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	152	Verschueren (1983)
Solubility	mg/l	16.1 (25°C)	Bodenschutz, 1988 (reference cannot be traced back)
Vapour pressure	Pa	0.89 (25°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	1.14 (25°C)	WHO (1998)
log Kow	g/g	4.07	WHO (1998)
log Koc	dm ³ /kg	3.79	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	5.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30x10 ⁻¹	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		Not evaluated D	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6x10 ⁻³	Carcinogenic potency = 0.01 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7x10 ⁻¹	Carcinogenic potency = 0.01 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6x10 ⁻³	= oral value
Limit value in air	mg/m ³	1.20x10 ⁻⁵	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	70	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	-	




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

- a) For the calculation of soil remediation values, BCF were filled in (2.32 mg/kg dm per mg/kg dm for all root and above ground vegetables).
- 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1.10^{-5}/(\text{dose at } 1.10^{-5} (\text{mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.3. ANTHRACENE










Parameter	Unit	Value	Source
CAS nr.		120-12-7	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	178	Verschueren (1983)
Solubility	mg/l	7.50×10^{-2} (15°C)	Verschueren (1983)
Vapour pressure	Pa	1.3×10^{-4}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	73 (25°C)	WHO (1998)
log Kow	g/g	4.45	van den Berg (1994)
log Koc	dm ³ /kg	4.59	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	5.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	-	
Diffusion coefficient water (Dw)	m ² /d	-	
Kp	[cm/h]	calculated	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 D	IARC (1998) Baars et al. (2001)
Systemic effects threshold			
TDI oral	mg/kg.d	3×10^{-1}	US-EPA (1994c)
TCL inhalation ^{b)}	mg/m ³	1.05	Nouwen et al. (2000)
TDI dermal	mg/kg.d	3×10^{-1}	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.05	From inhalation unit risk
Limit value in drinking water	mg/m ³	75	solubility
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	-	



Polycyclic Aromatic Hydrocarbons (PAHs)

Parameter	Unit	Value	Source
Dietary background adults	mg/kg day	4.00×10^{-7}	Vermeire et al. (1991)
Dietary background children	mg/kg.day	relative to adults (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/m ³	0	
Background indoor air	mg/m ³	0	 = outdoor air
Background drinking water	mg/m ³	0	

- a) For the calculation of soil remediation values, BCF were filled in (0.022 mg/kg dm per mg/kg dm above ground vegetables and 0.002 mg/kg dm per mg/kg dm for root vegetables).
- 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.

7.4. BENZO(A)ANTHRACENE

Parameter	Unit	Value	Source
CAS nr.		56-55-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	228	Verschuieren (1983)
Solubility	mg/l	1.00×10^{-2} (24°C)	Verschuieren (1983)
Vapour pressure	Pa	5.51×10^{-6}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	0.813 (25°C)	US-EPA (1994d)
log Kow	g/g	5.61	van den Berg (1994)
log Koc	dm ³ /kg	6.04	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	 ^{a)}
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	4.99×10^{-5}	?
Kp	[cm/h]	-	
FA	-	1	 US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	 US-EPA (2004)
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	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		2A B2	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	= oral value
Limit value in air	mg/m ³	1.20×10^{-6}	From inhalation unit risk
Limit value in drinking water	mg/m ³	7	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	-	


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

- a) For the calculation of soil remediation values, BCF were filled in (0.007 mg/kg dm per mg/kg dm above ground vegetables and 0.015 mg/kg dm per mg/kg dm for root vegetables).
- 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1 \cdot 10^{-5}/(\text{dose at } 1 \cdot 10^{-5} \text{ (mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.5. BENZO(A)PYRENE

Parameter	Unit	Value	Source
CAS nr.		50-32-8	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	252	Verschueren (1983)
Solubility	mg/l	3.00×10^{-3} (20°C)	Verschueren (1983)
Vapour pressure	Pa	1.31×10^{-8}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	0.034 (25°C)	WHO (1998)
log Kow	g/g	6.35	van den Berg (1994)
log Koc	dm ³ /kg	6.31	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	2.00×10^{-10}	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	4.75×10^{-5}	?
Kp	[cm/h]	calculated	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		2A B2	IARC (1998) US-EPA (1994a)
Systemic effects pseudo-threshold ^{b)}			
p-TDI oraal	mg/kg.d	2.2×10^{-5}	WHO (1998)
p-TCL inhalatoir ^{c)}	mg/m ³	5×10^{-7}	Background Flanders (OVAM, 2005a)
p-TDI dermaal	mg/kg.d	2.2×10^{-5}	= oral value
Limit value in air	mg/m ³	1.00×10^{-6}	Legal target value
Limit value in drinking water	mg/m ³	0.7	WHO (1998)
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	-	



Polycyclic Aromatic Hydrocarbons (PAHs)

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

- a) For the calculation of soil remediation values, BCF were filled in (0.002 mg/kg dm per mg/kg dm above ground vegetables and 0.012 mg/kg dm per mg/kg dm for root vegetables).
- b) The reference values were taken as provided in the substance sheets. As the reference value for inhalation does not correspond anymore to the toxicological value (and a unit risk cannot be used), the data are filled in as pseudo-threshold. This does not impact the calculations.
- c) 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.

7.6. BENZO(B)FLUORANTHENE

Parameter	Unit	Value	Source
CAS nr.		205-99-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	252	Verschueren (1983)
Solubility	mg/l	1.20×10^{-3} (20°C)	WHO (1998)
Vapour pressure	Pa	6.70×10^{-5} (20°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	5.1×10^{-2} (25°C)	WHO (1998)
log Kow	g/g	6.12	WHO (1998)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	?
Diffusion coefficient water (Dw)	m ² /d	4.75×10^{-5}	
Kp	[cm/h]	-	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		2B B2	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	= oral value
Limit value in air	mg/m ³	1.20×10^{-6}	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	1.2	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	-	




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

- a) For the calculation of soil remediation values, BCF were filled in (0.014 mg/kg dm per mg/kg dm above ground vegetables and 0.005 mg/kg dm per mg/kg dm for root vegetables).
- a) 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1.10^{-5}/(\text{dose at } 1.10^{-5} (\text{mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.7. BENZO(G,H,I)PERYLENE

Parameter	Unit	Value	Source
CAS nr.		191-24-2	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	276	Verschueren (1983)
Solubility	mg/l	2.60×10^{-4} (25°C)	Verschueren (1983)
Vapour pressure	Pa	2.59×10^{-9}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	2.7×10^{-2} (20°C)	calculated
log Kow	g/g	6	van den Berg (1994)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	0.8	US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 D	IARC (1998) Baars et al. (2001)
Systemic effects threshold			
TDI oral	mg/kg.d	3×10^{-2}	Baars et al. (2001)
TCL inhalation ^{b)}	mg/m ³	1.05×10^{-1}	calculated from oral value
TDI dermal	mg/kg.d	3×10^{-2}	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	1.05×10^{-1}	
Limit value in drinking water	mg/m ³	0.26	solubility
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	-	



Polycyclic Aromatic Hydrocarbons (PAHs)

Parameter	Unit	Value	Source
Dietary background adults	mg/kg day	2×10^{-6}	Vermeire et al. (1991)
Dietary background children	mg/kg.day	relative to adults (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/m ³	0	
Background indoor air	mg/m ³	0	 = indoor air
Background drinking water	mg/m ³	0	

- a) For the calculation of soil remediation values, BCF were filled in (0.004 mg/kg dm per mg/kg dm above ground vegetables and 0.011 mg/kg dm per mg/kg dm for root vegetables).
- 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.











7.8. BENZO(K)FLUORANTHENE



Parameter	Unit	Value	Source
CAS nr.		207-08-9	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	252	Verschueren (1983)
Solubility	mg/l	7.60×10^{-4} (25°C)	WHO (1998)
Vapour pressure	Pa	1.30×10^{-8} (20°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	4.40×10^{-2} (20°C)	WHO (1998)
log Kow	g/g	6.84	WHO (1998)
log Koc	dm ³ /kg	5.66	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	4.75×10^{-5}	?
Kp	[cm/h]	-	
FA	-	0.7	US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		2B B2	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	= oral value
Limit value in air	mg/m ³	1.20×10^{-6}	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	0.76	solubility
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	-	

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

- a) For the calculation of soil remediation values, BCF were filled in (0.003 mg/kg dm per mg/kg dm above ground vegetables and 0.015 mg/kg dm per mg/kg dm for root vegetables).
- 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1 \cdot 10^{-5} / (\text{dose at } 1 \cdot 10^{-5} \text{ (mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.9. CHRYSENE



Parameter	Unit	Value	Source
CAS nr.		218-01-9	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	228	Verschueren (1983)
Solubility	mg/l	1.50×10^{-3} (15°C)	Verschueren (1983)
Vapour pressure	Pa	2.6×10^{-7}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	calculated	
log Kow	g/g	6.64	van den Berg (1994)
log Koc	dm ³ /kg	5.72	WHO (1998)
Log Koa	g/g	-	
BCF		calculated	 a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	 US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	 US-EPA (2004)
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	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 B2	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-3}	Carcinogenic potency = 0.01 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7×10^{-1}	Carcinogenic potency = 0.01 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-3}	= oral value
Limit value in air	mg/m ³	1.20×10^{-5}	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	1.5	solubility
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	-	

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

- a) For the calculation of soil remediation values, BCF were filled in (0.008 mg/kg dm per mg/kg dm above ground vegetables and 0.013 mg/kg dm per mg/kg dm for root vegetables).
- 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1 \cdot 10^{-5}/(\text{dose at } 1 \cdot 10^{-5} \text{ (mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.10. DIBENZ(A,H)ANTHRACENE



Parameter	Unit	Value	Source
CAS nr.		53-70-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	278	Verschueren (1983)
Solubility	mg/l	5.00×10^{-4} (27°C)	WHO (1998)
Vapour pressure	Pa	1.30×10^{-8} (20°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	7.00×10^{-3} (25°C)	WHO (1998)
log Kow	g/g	6.5	WHO (1998)
log Koc	dm ³ /kg	6.31	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	5.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	5.00×10^{-10}	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	0.6	US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		2A B2	IARC (1998) Baars et al. (2001)
Systemic effects pseudo-threshold ^{b)}			
p-TDI oral	mg/kg.d	2.2×10^{-5}	relative Carcinogenic potency with regard to benzo(a)pyrene = 1
p-TCL inhalation ^{c)}	mg/m ³	2.5×10^{-7}	Background Flanders (OVAM, 2005a)
p-TDI dermal	mg/kg.d		= oral value
Limit value in air	mg/m ³	2.50×10^{-7}	background Flanders (OVAM, 2005a)
Limit value in drinking water	mg/m ³	0.4	solubility
Limit value in plants	mg/kg fw		
Limit value in meat			
Beef	mg/kg fw	-	
Mutton	mg/kg fw	-	
Liver	mg/kg fw	-	
Kidney	mg/kg fw	-	

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

- a) For the calculation of soil remediation values, BCF were filled in (0.0003 mg/kg dm per mg/kg dm above ground vegetables and 0.0005 mg/kg dm per mg/kg dm for root vegetables).
- b) The reference values were taken as provided in the substance sheets. As the reference value for inhalation does not correspond anymore to the toxicological value (and a unit risk cannot be used), the data are filled in as pseudo-threshold. This does not impact the calculations.
- c) 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

7.11. FENANTHRENE





Parameter	Unit	Value	Source
CAS nr.		85-01-8	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	178	Verschuere (1983)
Solubility	mg/l	1.60 (15°C)	Verschuere (1983)
Vapour pressure	Pa	2.41x10 ⁻³	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	3.98 (25°C)	WHO (1998)
log Kow	g/g	4.46	van den Berg (1994)
log Koc	dm ³ /kg	4.61	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	5.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	5.64x10 ⁻⁵	?
Kp	[cm/h]	-	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30x10 ⁻¹	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 D	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6x10 ⁻⁴	Carcinogenic potency = 0.001 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7x10 ⁻²	Carcinogenic potency = 0.001 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6x10 ⁻⁴	= oral value
Limit value in air	mg/m ³	1.20x10 ⁻⁴	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	120	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	-	

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

- a) For the calculation of soil remediation values, BCF were filled in (0.041 mg/kg dm per mg/kg dm above ground vegetables and 0.031 mg/kg dm per mg/kg dm for root vegetables).
- 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1 \cdot 10^{-5}/(\text{dose at } 1 \cdot 10^{-5} \text{ (mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.12. FLUORANTHENE

Parameter	Unit	Value	Source
CAS nr.		206-44-0	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	202	Verschuieren (1983)
Solubility	mg/l	2.65×10^{-1} (25°C)	Verschuieren (1983)
Vapour pressure	Pa	2.31×10^{-4}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	0.65 (20°C)	WHO (1998)
log Kow	g/g	5.33	van den Berg (1994)
log Koc	dm ³ /kg	5.21	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	5.30×10^{-5}	?
Kp	[cm/h]	calculated	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30E-01	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 D	IARC (1998) Baars et al. (2001)
Systemic effects threshold ^{b)}			Not included in the calculation of soil remediation values
TDI oral	mg/kg.d	4×10^{-2}	US-EPA (1994b)
TCL inhalation ^{c)}	mg/m ³	1.4×10^{-1}	calculated based on the TDI oral
TDI dermal	mg/kg.d	4×10^{-2}	= oral value
averaging period		child, adolescent, adult	
Systemic effects no threshold ^{d)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-3}	Carcinogenic potency = 0.01 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7×10^{-1}	Carcinogenic potency = 0.01 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-3}	= oral value
Limit value in air	mg/m ³	1.20×10^{-5}	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	4	WHO (1998) (1 % van TDI)



Parameter	Unit	Value	Source
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	5.00×10^{-6}	 SCF (2002) in Nouwen et al. (2000)
Dietary background children	mg/kg.day	relative to adults (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/m ³	0	
Background indoor air	mg/m ³	0	 = indoor air
Background drinking water	mg/m ³	0	

- a) For the calculation of soil remediation values, BCF were filled in (0.029 mg/kg dm per mg/kg dm above ground vegetables and 0.023 mg/kg dm per mg/kg dm for root vegetables).
- b) Fluoranthene is considered a carcinogen in the calculation of the soil remediation values. The report also gives values for the non-carcinogenic effects of pyrene. These are also taken up in the S-risk substance data sheet.
- c) 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.
- d) 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 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(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 m³/d (inhalation rate).

7.13. FLUORENE











Parameter	Unit	Value	Source
CAS nr.		86-73-7	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	166	Verschueren (1983)
Solubility	mg/l	1.98 (25°C)	WHO (1998)
Vapour pressure	Pa	0.08 (25°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	10.1 (25°C)	WHO (1998)
log Kow	g/g	4.18	WHO (1998)
log Koc	dm ³ /kg	4.39	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	5.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30x10 ⁻¹	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 D	IARC (1998) Baars et al. (2001)
Systemic effects threshold			
TDI oraal	mg/kg.d	4x10 ⁻²	US-EPA (1990)
TCL inhalatoir ^{b)}	mg/m ³	1.4x10 ⁻¹	Calculated on the basis of the oral TDI
TDI dermaal	mg/kg.d	4x10 ⁻²	= oral value
Limit value in air	mg/m ³	1.40x10 ⁻¹	
Limit value in drinking water	mg/m ³	120	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	-	



Polycyclic Aromatic Hydrocarbons (PAHs)

Parameter	Unit	Value	Source
Dietary background adults	mg/kg day	5.00×10^{-7}	WHO (1998)
Dietary background children	mg/kg.day	relative to adults (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/m ³	0	
Background indoor air	mg/m ³	0	 = outdoor air
Background drinking water	mg/m ³	0	

- a) For the calculation of soil remediation values, BCF were filled in (0.005 mg/kg dm per mg/kg dm above ground vegetables and 0.009 mg/kg dm per mg/kg dm for root vegetables).
- 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.

7.14. INDENO(1,2,3-CD)PYRENE

Parameter	Unit	Value	Source
CAS nr.		193-39-5	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	276	Verschueren (1983)
Solubility	mg/l	1.00×10^{-4} (11°C)	van den Berg (1994)
Vapour pressure	Pa	2.6×10^{-9}	van den Berg (1994)
Henry coefficient	Pa m ³ /mol	2.9×10^{-2} (20°C)	WHO (1998)
log Kow	g/g	7.43	van den Berg (1994)
log Koc	dm ³ /kg	calculated	
Log Koa	g/g	calculated	
BCF		calculated	 a)
Dpe	m ² /d	2.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	4.54×10^{-5}	
Kp	[cm/h]	calculated	
FA	-	0.6	 US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	 US-EPA (2004)
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	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	 Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		2B B2	IARC (1998) Baars et al. (2001)
Systemic effects no threshold ^{b)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7	Carcinogenic potency = 0.1 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-2}	= oral value
Limit value in air	mg/m ³	1.20×10^{-6}	calculated from inhalation unit risk
Limit value in drinking water	mg/m ³	0.1	solubility
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	-	



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

- a) For the calculation of soil remediation values, BCF were filled in (0.0001 mg/kg dm per mg/kg dm above ground vegetables and 0.0002 mg/kg dm per mg/kg dm for root vegetables).
- 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 $((\text{mg}/\text{kg}\cdot\text{d})^{-1}) = 1 \cdot 10^{-5} / (\text{dose at } 1 \cdot 10^{-5} \text{ (mg}/\text{kg}\cdot\text{d}))$. 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 m³/d (inhalation rate).

7.15. NAPHTHALENE

Parameter	Unit	Value	Source
CAS nr.		91-20-3	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	128	Verschueren (1983)
Solubility	mg/l	30 (20°C)	Verschueren (1983)
Vapour pressure	Pa	32 (25°C)	Perry en Green (1984)
Henry coefficient	Pa m ³ /mol	48.9 (25°C)	
log Kow	g/g	3.36	van den Berg (1994)
log Koc	dm ³ /kg	3.17	WHO (1998)
Log Koa	g/g	calculated	
BCF		calculated	a)
Dpe	m ² /d	5.00x10 ⁻⁷	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	0.5544	van den Berg (1994)
Diffusion coefficient water (Dw)	m ² /d	6.65x10 ⁻⁵	?
Kp	[cm/h]	calculated	
FA	-	1	US-EPA (2004)
ABS dermal soil/dust	-	1.30x10 ⁻¹	US-EPA (2004)
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	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		Not evaluated D/C	IARC (1998) US-EPA, 1993 (IRIS-online, cannot be traced back
Systemic effects threshold			
TDI oral	mg/kg.d	2x10 ⁻²	US-EPA (1998)
TCL inhalation ^{b)}	mg/m ³	3x10 ⁻³	US-EPA (1998)
TDI dermal	mg/kg.d	2x10 ⁻²	= oral value
averaging period		child, adolescent, adult	
Limit value in air	mg/m ³	3.00x10 ⁻³	US-EPA (1998)
Limit value in drinking water	mg/m ³	60	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	-	

Polycyclic Aromatic Hydrocarbons (PAHs)

Parameter	Unit	Value	Source
Egg	mg/kg fw	-	
Dietary background adults	mg/kg day	2.90×10^{-3}	Hassauer et al. (1993)
Dietary background children	mg/kg.day	relative to adults (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/m ³	9.50×10^{-4}	ATSDR (1995)
Background indoor air	mg/m ³	9.50×10^{-4}	 = outdoor air
Background drinking water	mg/m ³	0	

- a) For the calculation of soil remediation values, BCF were filled in (2.92 mg/kg dm per mg/kg dm above ground vegetables and 2.92 mg/kg dm per mg/kg dm for root vegetables).
- 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.

7.16. PYRENE

Parameter	Unit	Value	Source
CAS nr.		129-00-0	
Type		organic	
Dissociating		no	
Molecular weight	g/mol	202	Verschueren (1983)
Solubility	mg/l	1.35×10^{-1} (25°C)	WHO (1998)
Vapour pressure	Pa	6.00×10^{-4} (25°C)	WHO (1998)
Henry coefficient	Pa m ³ /mol	1.10 (25°C)	WHO (1998)
log Kow	g/g	5.18	WHO (1998)
log Koc	dm ³ /kg	4.88	WHO (1998)
Log Koa	g/g	calculated	☒
BCF		calculated	☒ ^{a)}
Dpe	m ² /d	5.00×10^{-7}	van den Berg (1994)
Dpvc	m ² /d	calculated	
Diffusion coefficient air (Da)	m ² /d	calculated	
Diffusion coefficient water (Dw)	m ² /d	calculated	
Kp	[cm/h]	calculated	☒
FA	-	1	☒ US-EPA (2004)
ABS dermal soil/dust	-	1.30×10^{-1}	☒ US-EPA (2004)
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	☒ Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
BTF feed - egg	d/kg	0	☒ Low recovery in egg yolk in investigated PAHs (Fournier, et al., 2010)
Carcinogenicity		3 D	IARC (1998) Baars et al. (2001)
Systemic effects threshold ^{b)}			☒ Not included in the calculation of soil remediation values
TDI oral	mg/kg.d	3×10^{-2}	
TCL inhalation ^{c)}	mg/m ³	1.05×10^{-1}	Calculated from oral value
TDI dermal	mg/kg.d	3×10^{-2}	= oral value
averaging period		child, adolescent, adult	
Systemic effects no threshold ^{d)}			
Oral slope factor	(mg/kg.d) ⁻¹	4.6×10^{-4}	Carcinogenic potency = 0.001 with regard to benzo(a)pyrene
Inhalation unit risk	(mg/m ³) ⁻¹	8.7×10^{-2}	Carcinogenic potency = 0.001 with regard to benzo(a)pyrene
Dermal slope factor	(mg/kg.d) ⁻¹	4.6×10^{-4}	= oral value
Limit value in air	mg/m ³	1.20×10^{-4}	calculated from inhalation unit risk

Parameter	Unit	Value	Source
Limit value in drinking water	mg/m ³	90	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	5.00x10 ⁻⁶	SCF (2002) in Nouwen et al. (2000)
Dietary background children	mg/kg.day	relative to adults (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/m ³	0	
Background indoor air	mg/m ³	0	= outdoor air
Background drinking water	mg/m ³	0	

- a) For the calculation of soil remediation values, BCF were filled in (0.011 mg/kg dm per mg/kg dm above ground vegetables and 0.021 mg/kg dm per mg/kg dm for root vegetables).
- b) Pyrene is considered a carcinogen in the calculation of the soil remediation values. The report also gives values for the non-carcinogenic effects of pyrene. These are also taken up in the S-risk substance data sheet.
- c) 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
- d) 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 1/10⁵. S-Risk uses slope factors and unit risks. Conversion is as follows: slope factor ((mg/kg.d)⁻¹) = 1.10⁻⁵/(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 m³/d (inhalation rate).

REFERENCES

- ATSDR. (1995). Toxicological Profile Polycyclic Aromatic Hydrocarbons.
- Baars, A. J., Theelen, R. M. C., Janssen, P. J. C. M., Hesse, J. M., van Apeldoorn, M. E., Meijerink, M. C. M., Verdam, L., & Zeilmaker, M. J. (2001). Re-evaluation of human-toxicological maximum permissible risk levels.
- 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.
- Fournier, A., Feidt, C., Dziurla, M.-A., Grandclaoudon, C., & Jondreville, C. (2010). Transfer kinetics to egg yolk and modeling residue recovered in yolk of readily metabolized molecules: polycyclic aromatic hydrocarbons orally administered to laying hens. *Chemosphere*, 78, 1004-1010.
- Hassauer, M., Kalberlach, F., Oltmanns, J., & Schneider, K. (1993). Basisdaten Toxikologie für umweltrelevante Stoffe zur Gefahrenbeurteilung bei Altlasten.
- IARC. (1998). Polynuclear aromatic compounds Part 1, Chemical, Environmental and Experimental Data - summary of data reported and evaluation. *Volume 32*.
- Nouwen, J., Cornelis, C., Provoost, J., Schoeters, G., Weltens, R., & Patyn, J. (2000). Voorstel tot normering van de bodemsaneringsnormen voor PAK.
- 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 gechlloreerde 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.
- Perry, R. H., & Green, D. (1984). *Perry's chemical engineer handbook* (6th edition ed.): Mc Grawhill.
- SCF. (2002). Opinion of the Scientific Committee on food on the risks to human health of Polycyclic Aromatic Hydrocarbons in food.
- US-EPA. (1990). IRIS - Fluorene (CAS n° 86-73-7).
- US-EPA. (1991). IRIS - Acenaphhtylene (CAS n° 208-96-8).
- US-EPA. (1994a). IRIS - Benzo(a)pyrene (CAS n° 50-35-8).
- US-EPA. (1994b). IRIS - Fluoranthene (CAS n° 206-44-0).
- US-EPA. (1994c). IRIS -Anthracene (CAS n° 120-12-7).
- US-EPA. (1994d). Technical background document for Draft Soil Screening Level Guidance.

- US-EPA. (1998). IRIS - Naphthalene (CAS n° 91-20-3).
- 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. (1994). Blootstelling van de mens aan bodemverontreiniging. Een kwalitatieve en kwantitatieve analyse, leidend tot voorstellen voor humaan toxicologische C-toetsingswaarden (beperkt herziene versie).
- Vermeire, T. G., Apeldoorn, M. E., Fouw, J. C., & Janssen, P. J. C. M. (1991). Voorstel voor de humaantoxicologische onderbouwing van C-(toetsings)waarden.
- Verschueren, K. (1983). *Handbook of environmental data on organic chemicals*. New York, VS: Van Nostrand Reinhold.
- WHO. (1998). Selected non-heterocyclic polycyclic aromatic hydrocarbons. *Environmental Health Criteria*.