

Final report

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

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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 |
| 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 | Verschuere (1983) |
| Solubility | mg/l | 1.00×10^{-2} (24°C) | Verschuere (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 | Verschueren (1983) |
| Solubility | mg/l | 1.60 (15°C) | Verschueren (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) |

Polycyclic Aromatic Hydrocarbons (PAHs)



| 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 | Verschuere (1983) |
| Solubility | mg/l | 30 (20°C) | Verschuere (1983) |
| Vapour pressure | Pa | 32 (25°C) | Perry and 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 gechloreerde koolwaterstoffen (1,2-DCA, VC, CHL en HCB): stofdata.
- OVAM. (2009c). Aanvulling bij basisinformatie voor risico-evaluaties - zware metalen en arseen: stofdata.
- OVAM. (2009d). Rekenmodule voor de opname van zware metalen in planten en transfer naar de voedselketen.
- 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*.