



REPORT

Oppdatering av stoffdata for forbindelser i forurensset grunn

UPDATING OF BACKGROUND DATA FOR
COMPOUNDS IN CONTAMINATED SOIL

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Summary

The Norwegian Geotechnical Institute (NGI) has reviewed the existing compound specific data that are used in risk assessment of contaminated soil. This is the first such revision since 2007 for most substances. Since 2007, there have been several substantial advances regarding data availability within Europe. This includes the revision of the European Union's and Norway's Water Framework Directive, the implementation of REACH (The Registration, Evaluation, Authorisation and Restriction of Chemicals), new chemicals of concern being prioritized, improved analytical techniques and the publication of several new risk assessment reports and studies on soil contamination. This report considers these new advances in reviewing the compound specific data that are used to predict fate and transport of the contaminants as well as their potential risk. The data reported here were collected in 2016, for PFOS and PFOA data were revised in the autumn of 2019 and a recent proposal from the European Food Safety Authority on PFAS (24-02-2020) was included in the data compilation.

Compound specific data for the following new compounds not previously included in the risk assessment framework have been compiled:

- ↗ D5
- ↗ PFOA
- ↗ Triclosane
- ↗ TCEP
- ↗ Dodecylphenols
- ↗ Diuron
- ↗ Irgarol
- ↗ Antimony
- ↗ Galaxolide
- ↗ Tonalide
- ↗ Sum trichlorobenzenes (instead of 1,2,4-trichlorobenzene, 1,2,3-trichlorobenzene and 1,3,5-trichlorobenzene as done previously, individually, to be consistent with Water Framework Directive 2013/39 EU and Norway's updated sediment and water quality standards M-608/2016)
- ↗ Brominated diphenyl ethers as the sum of BDE 28, 47, 99, 100, 153 and 154 (instead of just BDE 99 and BDE 154 individually, again to be consistent with Directive 2013/39 EU and M-608/2016)

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Review and reference page

1 Introduction

The Norwegian Environment Agency (Miljødirektorat) first introduced a system for risk assessment of contaminated soil in the 1999 guideline "Veileddning om risikovurdering av forurensset grunn" (TA-1629/1999). This guideline used compound specific data to describe expected fate and transport of the contaminants as well as their potential risk for humans and the environment. In 2007, a suggestion for revision was introduced based on the latest available data at that time, and included a new list of substances, such as brominated flame retardants, PFOS, chlorinated paraffins, alkyl-phenols and phthalates (Aquateam 2007), which were later put into effect in a revision of the risk assessment tool. In 2013, organotin substances were also added (Aquateam 2011).

This report presents a further revision of the compound specific data conducted by the Norwegian Geotechnical Institute (NGI) in 2016 (PFOS and PFOA data were revised in 2019). Compound specific data were reviewed and updated with the newest data, particularly in relation to the EU Water Framework Directive (Directive 2013/39 EU) updated in August 2013, and the Norwegian water and sediment guideline concentrations updated in 2016 (M-608/2016). This included the following new substances not previously included in terrestrial risk assessment in Norway:

- ↗ D5
- ↗ PFOA
- ↗ Triclosane
- ↗ TCEP
- ↗ Dodecylphenols
- ↗ Diuron
- ↗ Irgarol
- ↗ Antimony
- ↗ Galaxolide
- ↗ Tonalide
- ↗ Sum trichlorobenzenes (instead of 1,2,4-trichlorobenzene, 1,2,3-trichlorobenzene and 1,3,5-trichlorobenzene, individually, to be consistent with Directive 2013/39 EU and M-608/2016)
- ↗ Brominated diphenyl ethers as the sum of BDE 28, 47, 99, 100, 153 and 154 (instead of just BDE 99 and BDE 154 individually, to be consistent with Directive 2013/39 EU and M-608/2016)
- ↗ Sum nonylphenols and their ethoxylates (as nonylphenolethoxylates eventually degrade to nonylphenols)
- ↗ Sum octylphenols and their ethoxylates (as octylphenolethoxylates eventually degrade to octylphenols)

The following substance was not revised due to lack of data:

- ↗ 1,2,4,5-tetrachlorbenzene

2 Methodology of deriving compound specific data

2.1 Relevant parameters

The key chemical background parameters needed to be able to calculate human health risk following the Norwegian guideline for risk assessment of human health are listed in (Table 1). All these parameters were included in the literature review for updating and revision.

Table 1 Overview of properties needed to derive QS_{soil}(human health)

Parameter	Definition	Comments
log Pow (l/l)	Octanol-water partition coefficient	Not relevant for metals
Koc(l/kg TS)	Organic carbon-water partition coefficient	Not relevant for metals; in many cases it is estimated from log Pow
K_D(l/kg TS)	Soil-water distribution coefficient	Directly measured for metals. Estimated here for organic compounds as 0.01 Koc, based on the assumption that typical Norwegian soil is 1% organic carbon (OC)
Henry (-)	Henry's law coefficient	Describes air-water transfer
BCF fish (l/kg w.w.)	Bioconcentration factor in fish	If not available from the literature it is estimated according to equation 1
BCF stem (l/kg w.w.)	Bioconcentration factor in plant stems	If not available from the literature it is estimated from equation 2
BCF root (l/kg w.w.)	Bioconcentration in plant roots	If it is not available from the literature it is estimated from equation 3
MTDI (mg/kg/d)	Maximum tolerable daily intake	For human toxicity
MTDI cancer (mg/kg/d)	Maximum tolerable daily intake for a carcinogen	For human toxicity
RfC (mg/m³)	Toxic reference concentration (air)	For human toxicity
RfC cancer (mg/m³)	Toxic reference concentration for mutagenic/ carcinogenic substances	For human toxicity
Skin contact: f_{du}	Dermal absorption factor	For human toxicity

2.2 Estimating parameters

In the absence of applicable literature data on specific parameters, values have been estimated using the equations derived from the Norwegian risk assessment guideline (SFT, 1999) and given below:

Equation 1:

$$\begin{aligned}\log \text{BCF}_{\text{fish}} &= 0.85 \log \text{Pow} - 0.7 && (\log \text{Pow from 2 to } 6) \\ \log \text{BCF}_{\text{fish}} &= -0.2(\log \text{Pow})^2 + 2.74 \log \text{Pow} - 4.72 && (\text{for } \log \text{Pow} > 6)\end{aligned}$$

Equation 2:

$$\text{BCF}_{\text{stem}} = 0.784(0.82 + 10^{0.95\log\text{Pow} - .05})\left(10^{-0.434\frac{(\log\text{Pow}-1.78)^2}{2.44}}\right)$$

Equation 3:

$$\text{BCF}_{\text{root}} = 10^{(0.77\log\text{Pow}-1.52)} + 0.82$$

Soil-water partition coefficient, K_D in this report are presented for a "typical Norwegian" soil with 1% OC (dry weight) following the description in the Norwegian risk assessment guideline (SFT, 1999).

3 Approach for reviewing of available literature

Within Europe there has been several new advances in how environmental risk is regulated this has generated several new data sets to consider, since the last time the compound specific data were evaluated in 2007.

Some of the key developments are:

- The Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation of EU, which requires producers and importers of chemicals, under certain conditions, to provide toxicity, ecotoxicity and physical chemical data to register their chemicals in Europe. The data base of REACH registered chemicals has compiled thousands of physical-chemical properties and toxicity studies (<https://echa.europa.eu/information-on-chemicals/registered-substances>).
- Several new ecotoxicity studies and risk assessment reports at the national, European and international level have been published.

A feature of these developments is that there is a European-wide centralized assembly of key physical-chemical property data, and evaluation of toxicity studies. This makes it possible to coordinate the use of background data used for risk assessment across different European countries. This is in contrast to earlier times, in the absence of such centralized data base, when individual studies put together their own compilations of data. To make good use of this it was key that the background parameters used here were as synchronized as possible to the recently published water and sediment quality guideline values in Norway (M-241, M-608), as well as the water framework directive (2013/39 EU). Therefore the sources for new information were obtained using the priority presented in Table 9.

Table 9. Overview of parameters presented.

Priority	Types of Sources
1.	Background reports to the EU water framework directive (Directive 2013/39 EU) and new Norwegian EQS values (M-608/2016) for water and sediments
2.	Newest EU risk assessment reports (EQS dossier, EU RAR, SVHC dossiers, etc., national reports), recent Norwegian reports (after 2007), or the peer-reviewed literature
3.	Data obtained from the REACH registration dossiers https://echa.europa.eu/information-on-chemicals/registered-substances
4.	Previous data from Aquateam 2007 and 2011.

Data from all four types of sources were compiled in the preparation of this report, but only data corresponding to the highest priority in the table above is presented.

Regarding the REACH data, only human toxicology data from the "toxicological summary" section of the "toxicological summary" was considered, with the exception of dermal absorption factor(f_{du}) which was acquired from the dermal absorption datasheet (within the toxicokinetics, metabolism and distribution data sheet within the toxicological information). Other data was obtained from the "Physical & chemical property" and "Environmental fate & pathways" data bases.

REACH data is also registered with a reliability score, with a score of 1 meaning "reliable without restriction", 2 "reliable with restrictions", 3 "not reliable" and 4 "not assignable". As there are no real rules to guide what reliability score to assign, and it is often up to the opinion of the REACH registrant, it is difficult to ascertain the relationship of this reliability score with data quality. Nevertheless, the reliability scores were provided for data obtained from the REACH registration dossiers.

4 Revised compound specific data

Data are presented for each of the compounds in a table that provides background parameters and concentrations. New data under the column "new review" is presented in bold, blue font. Otherwise data in this column is the same as previous values from Aquateam (2007) and Aquateam (2011).

4.1 Arsenic

Background Parameters and Concentrations

Substance	Arsenic		
CAS #		7440-38-2	
M.W. (g/mol)		75	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K _D (l/kg TS)	100	6607	UK Environment Agency (As)
Henry (-)	-	-	
BCF fish (l/kg w.w.)	50	4	UK Environment Agency (As): 4 (fish), 12 (snegl), 140 - 3688 (algæ og planter)
BCF stem	0.03	0.03	
BCF root	0.015	0.015	
MTDI (mg/kg/d)	0.001	0.0003	REACH As(III) = 0.0022; 30% of TDI in RIVM (2001) = 0.0003
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	0.0025	REACH (AS(III) chronic = 0.0025)
RfC cancer (mg/m ³)	0.00000067	0.00000067	
Skin contact: f _{du}	0.03	0.03	
Background			
Freshwater (µg/L)	-	0.15	TA-2361 (slightly above average of 0.134 µg/L)
Coastal water (µg/L)	-	0.15	TA-2361 (slightly above average of 0.134 µg/L)
Sediment (mg/kg)	-	15	OSPAR (2006)
Soil (mg/kg)	0.07-58	4.9	TA-2863 median natural background Oslo & Trondheim

4.2 Lead

Background Parameters and Concentrations

Substance	Lead		
CAS #		7439-92-1	
M.W. (g/mol)		207	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K_D(l/kg TS)	1000	154882	EU dossier (Pb)
Henry (-)	-	-	
BCF fish (l/kg w.w.)	300	424	median in EU dossier (Pb)
BCF stem	0.03	0.03	
BCF root	0.001	0.001	
MTDI (mg/kg/d)	0.00105	0.00108	30% of TDI in RIVM (2001) = 0.00108
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.00015	0.00015	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.006	0.0009	REACH Reliability 2, exp, median used (0,0005; 0,0013)
Background			
Freshwater (µg/L)	-	0.02	EU dossier (Pb)
Coastal water (µg/L)	-	0.02	EU dossier (Pb)
Sediment (mg/kg)	-	25	Ospar (2006), similar to EU dossier (Pb)
Soil (mg/kg)	5-157	10.25	TA-2863 median natural background Oslo & Trondheim

4.3 Cadmium

Background parameters and concentrations

Substance	Cadmium		
CAS #		7440-43-9	
M.W. (g/mol)		112	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K_D(l/kg TS)	100	130000	dependant on CO ₃ and salt cons.
Henry (-)	-	-	
BCF fish (l/kg w.w.)	200	623	EU dossier (Cd) worst case: BCF from 0.51 to 623 (whole fish)
BCF stem	0.7	0.7	
BCF root	0.15	0.15	
MTDI (mg/kg/d)	0.000125	0.00015	30% of TDI in RIVM (2001) = 0.00015; REACH chronic = 0.001
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.000005	0.000005	
RfC cancer (mg/m³)	0.0000056	0.0000056	
Skin contact: f_{du}	0.14	0.14	
Background			
Freshwater (µg/L)	-	0.003	EU dossier (Cd) (dissolved)
Coastal water (µg/L)	-	0.025	EU dossier (Cd) for marine vann
Sediment (mg/kg)	-	0.2	Ospar (2006)
Soil (mg/kg)	<0.01-1.8	0.065	TA-2863 median natural background Oslo & Trondheim

4.4 Mercury

Background parameters and concentrations

Substance	Mercury		
CAS #		7439-97-6	
M.W. (g/mol)		201	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K_D(l/kg TS)	500	100000	
Henry (-)	0.3	0.3	
BCF fish (l/kg w.w.)	200	200	Variable EU dossier (Hg)
BCF stem	0.03	0.03	
BCF root	0.015	0.015	
MTDI (mg/kg/d)	0.0001	0.00222	30% of REACH chronic value of 0.0074 (other values: RIVM (2001) - 0.0001 organic; EU dossier (Hg) 0.00047 organic (0.00071 total))
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.001	0.004	REACH
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.05	0.05	
Background			
Freshwater (µg/L)	-	0.001	EU dossier (Hg)
Coastal water (µg/L)	-	0.001	EU dossier (Hg)
Sediment (mg/kg)	-	0.05	Ospar (2006)
Soil (mg/kg)	0.005-0.2	0.210	TA-2863 median of maximum natural background values in different areas of Norway (ranging from 0.1 to 0.45)

4.5 Copper

Background parameters and concentrations

Substance	Copper		
CAS #		7440-50-8	
M.W. (g/mol)		64	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K_D(l/kg TS)	500	24409	
Henry (-)	-	-	
BCF fish (l/kg w.w.)	200	200	<i>Variable</i> very uncertain (varies with soil properties) EU RAR (Cu)
BCF stem	0.1	0.1	
BCF root	0.1	0.1	
MTDI (mg/kg/d)	0.5	0.163	RIVM (2001) = 140 µg/kg/d; EU RAR (Cu b) = 163 µg/kg/d
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.02	0.112	REACH Reliability 1 exp, median used (0,098; 0,157; 0,193; 0,128; 0,126; 0,147; 0,086; 0,046; 0,097; 0,136; 0,038)
Background			
Freshwater (µg/L)	-	0.3	TA-2361
Coastal water (µg/L)	-	0.3	TA-2361
Sediment (mg/kg)	-	20	
Soil (mg/kg)	1-246	29	TA-2863 median natural background Oslo & Trondheim

4.6 Zinc

Background parameters and concentrations

Substance	Zinc		
CAS #		7440-66-6	
M.W. (g/mol)		65	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K_D(l/kg TS)	200	110000	Kd 110000 used the most in EU RAR (Zn)
Henry (-)	-	-	
BCF fish (l/kg w.w.)	1000	1000	Variable no value suggested in EU RAR (Zn)
BCF stem	0.4	0.4	
BCF root	0.1	0.1	
MTDI (mg/kg/d)	0.3	0.5	RIVM (2001) = 0.5; REACH chronic = 0.83
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	2.5	REACH = 2.5
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.02	0.02	
Background			
Freshwater (µg/L)	-	1.5	TA-2803
Coastal water (µg/L)	-	1.5	TA-2803
Sediment (mg/kg)	-	90	OSPAR (2006)
Soil (mg/kg)	1.7-1000	80	TA-2863 median natural background Oslo & Trondheim

4.7 Chromium (III)

Background parameters and concentrations

Substance	Chromium (III)		
CAS # M.W. (g/mol)	10588-01-9 (Na ₂ Cr ₂ O ₇); 7789-09-5 ((NH ₄) ₂ Cr ₂ O ₇); 7778-50-9 (K ₂ Cr ₂ O ₇) 52		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
K _{oc} (l/kg TS)	-	-	
K _D (l/kg TS)	2000	<i>11000</i>	EU RAR (Cr), veldig variabelt med pH, redox, og andre parameter.
Henry (-)	-	-	
BCF fish (l/kg w.w.)	200	200	
BCF stem	0.02	0.02	
BCF root	0.002	0.002	
MTDI (mg/kg/d)	1	<i>0.0015</i>	30% of TDI in RIVM (2001) = 0.0015
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	<i>0.5</i>	REACH
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.04	0.04	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	2.6-246	<i>46.5</i>	TA-2863 median natural background Oslo & Trondheim (total Cr)

4.8 Chromium (VI)

Background parameters and concentrations

Substance	Chromium (VI)		
CAS # M.W. (g/mol)	1333-82-0 (CrO ₃); 7775-11-3 (Na ₂ CrO ₄); 52		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K _D (l/kg TS)	30	30	
Henry (-)	-	-	
BCF fish (l/kg w.w.)	200	200	
BCF stem	0.02	0.02	
BCF root	0.002	0.002	
MTDI (mg/kg/d)	0.003	0.0015	30% of TDI in RIVM (2001) = 0.0015
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	0.000008	0.000008	
RfC cancer (mg/m ³)	0.00000025	0.00000025	
Skin contact: f _{du}	0.09	0.09	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	<0.01-0.09	<0.01-0.09	

4.9 Chromium total (III + VI)

Background parameters and concentrations

Substance	Chromium total (III + VI)			
	CAS #	2007 Values	New Review	References for new values and notes
CAS #		7440-47-3 (Cr metall)		
M.W. (g/mol)		52		
Property	2007 Values	New Review	References for new values and notes	
log Pow (l/l)	-	-		
Koc(l/kg TS)	-	-		
KD(l/kg TS)	30	11000	EU RAR (Cr), veldi variable med pH, redox, og andre parameter. Verdi presentert er for Cr(III), fordi mest Cr i sediment skal være redusert til Cr(III).	
Henry (-)	-	-		
BCF fish (l/kg w.w.)	200	50	fish: 1 (Cr III), 100 (Cr IV) variable (pH and species dependent, shellfish 2800 - 9100, alga 500 - 130000)	
BCF stem	0.002	0.002		
BCF root	0.02	0.02		
MTDI (mg/kg/d)	1	0.0015	30% of TDI in RIVM (2001) for Cr(VI) or Cr(III) = 0.0015	
MTDI cancer (mg/kg/d)	-	-		
RfC (mg/m³)	0.00005	0.027	REACH local = 0.027	
RfC cancer (mg/m³)	0.0000003	0.0000003		
Skin contact: f_{du}	0.09	0.09		
Background				
Freshwater (µg/L)	-	0.1	TA-2361 (slightly above average of 0.09 µg/L)	
Coastal water (µg/L)	-	0.1	TA-2361 (slightly above average of 0.09 µg/L)	
Sediment (mg/kg)	-	60	OSPAR (2006)	
Soil (mg/kg)	2.6-246	46.5	TA-2863 median natural background Oslo & Trondheim	

4.10 Nickel

Background parameters and concentrations

Substance	Nickel		
CAS #	7440-02-0		
M.W. (g/mol)	59		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K_D(l/kg TS)	200	7079	
Henry (-)	-	-	
BCF fish (l/kg w.w.)	100	270	for bivalves EQS Dossier (Ni)
BCF stem	0.1	0.1	
BCF root	0.07	0.07	
MTDI (mg/kg/d)	0.005	0.015	30% of TDI in RIVM (2001) = 0.05; EU dossier (Ni) = 0.015; REACH chronic = 0.02 (acute = 0.012)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.000025	0.000025	
RfC cancer (mg/m³)	0.000012	0.000012	
Skin contact: f_{du}	0.35	0.35	
Background			
Freshwater (µg/L)	-	0.5	EU dossier (Ni)
Coastal water (µg/L)	-	0.5	EU dossier (Ni)
Sediment (mg/kg)	-	30	Ospar (2006) = 30, EU dossier (2011) median = 33
Soil (mg/kg)	2-1100	42.5	TA-2863 median natural background Oslo & Trondheim

4.11 Cyanide

Background parameters and concentrations

Substance	free cyanide		
CAS #		57-12-5	
M.W. (g/mol)		26.02	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-0.25	REACH Reliability 2 (20 °C)
Koc(l/kg TS)	-	2.8	REACH Reliability 2 (estimated)
K_D(l/kg TS)	1	0.028	0.01 Koc
Henry (-)	0.0013	0.005	REACH Reliability 2
BCF fish (l/kg w.w.)	10	0.12	calculated EU-TGD (2011)
BCF stem	0.883	0.12	based on new Pow
BCF root	0.798	0.84	based on new Pow
MTDI (mg/kg/d)	0.012	0.012	
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.025	0.025	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.3	0.3	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	m.d	m.d	

4.12 PCB 7

Background parameters and concentrations

Substance	PCB 7		
CAS #		1336-36-3	
M.W. (g/mol)		375.7 (average)	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6	5.7	ATSDR (1997, from 4.7 to 6.8:
Koc(l/kg TS)	500000	321119	
K_D(l/kg TS)	-	3211	0.01 Koc
Henry (-)	0.00034	0.00034	
BCF fish (l/kg w.w.)	47000	24950	average saltwater fish
BCF stem	200	200	estimated value = 3
BCF root	200	200	estimated value = 763
MTDI (mg/kg/d)	0.000003	0.00001	RIVM (2001) as non-planar PCBs = 0.00001
MTDI cancer (mg/kg/d)	0.0000013	0.0000013	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.067	0.067	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-	0.0003	
Soil (mg/kg)	0.00002-0.00014	0.00002-0.00014	OSPAR (2006)

4.13 Lindane

Background parameters and concentrations

Substance	lindane		
CAS #	608-73-1		
M.W. (g/mol)	291		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.61	3.5	EU dossier (HCH)
Koc(l/kg TS)	1080	3715	variable (650 - 7000)
K_D(l/kg TS)	33	37	0.01 Koc
Henry (-)	0.00000292	0.00000292	
BCF fish (l/kg w.w.)	730	1300	whole fish
BCF stem	0.15	0.15	estimated value = 5
BCF root	0.86	0.86	estimated value = 16
MTDI (mg/kg/d)	0.00033	0.001	RIVM (2001) (1 for α-HCH, 0.02 for β-HCH, and 0.04 for lindane) = 0.001
MTDI cancer (mg/kg/d)	0.0000075	0.0000075	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.000026	0.000026	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	0.002-0.03	0.002-0.03	

4.14 DDT

Background parameters and concentrations

Substance	DDT		
CAS # M.W. (g/mol)		50-29-3 for p,p-DDT 354	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.2	6.91	p,p-DDT (EPI Suite)
Koc(l/kg TS)	408600	6215857	eq
K_D(l/kg TS)	4086	62159	0.01 Koc
Henry (-)	0.0023	0.0023	
BCF fish (l/kg w.w.)	30000	30000	12000 – 100000 USDHHS (2002),
BCF stem	0.05	0.05	estimated value = 1
BCF root	0.002	0.002	estimated value = 6321
MTDI (mg/kg/d)	0.0005	0.01	0.01 from TA-2802; RIVM (2001) = 0.0005
MTDI cancer (mg/kg/d)	0.000029	0.000029	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.007	0.007	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-	0	0
Coastal water (µg/L)	-	0	0
Sediment (mg/kg)	-	0	0
Soil (mg/kg)	0.0003-0.02	0.0003-0.02	

4.15 Monochlorobenzene

Background parameters and concentrations

Substance	monochloro-benzene		
CAS # M.W. (g/mol)		108-90-7 113	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.9	2.89	REACH Reliability 2
Koc(l/kg TS)	219	398	REACH Reliability 4 (median 2.68;2.52)
KD(l/kg TS)	2.2	4	0.01 Koc
Henry (-)	0.13	0.15	REACH (reliability not given)
BCF fish (l/kg w.w.)	40	57	calculated EU-TGD (2011)
BCF stem	2.48	2.74	
BCF root	5.07	5.89	
MTDI (mg/kg/d)	0.02	0.2	RIVM (2001) = 0.2; REACH acute = 3
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	1	REACH
RfC cancer (mg/m³)	0.071	0.071	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.16 1,2-dichlorobenzene

Background parameters and concentrations

Substance	1,2-dichlorobenzene		
CAS # M.W. (g/mol)		95-50-1 147	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.5	3.43	REACH Reliability 2
Koc(l/kg TS)	398	398	
KD(l/kg TS)	4	4	0.01 Koc
Henry (-)	0.058	0.079	REACH (reliability not given)
BCF fish (l/kg w.w.)	230	164	calculated EU-TGD (2011)
BCF stem	4.41	4.37	
BCF root	14.4	14.0	
MTDI (mg/kg/d)	0.43	0.43	RIVM (2001) = 0.43; REACH chronic = 0.6 (acute = 3)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	1	REACH chronic = 1; (acute = 5)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.17 1,4-dichlorobenzene

Background parameters and concentrations

Substance	1,4-dichlorobenzene		
CAS # M.W. (g/mol)	106-46-7 147		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.5	3.37	REACH Reliability 2
Koc(l/kg TS)	661	372	REACH Reliability 2 (median 2.56 - 2.58)
KD(l/kg TS)	6.6	3.7	0.01 Koc
Henry (-)	0.093	0.10	REACH Reliability 2
BCF fish (l/kg w.w.)	1800	146	calculated EU-TGD (2011)
BCF stem	4.31	4.17	
BCF root	13.6	12.7	
MTDI (mg/kg/d)	0.11	0.1	RIVM (2001) = 0.1; REACH chronic = 0.7 (acute = 3.5)
MTDI cancer (mg/kg/d)	0.0004	0.0004	
RfC (mg/m ³)	0.13	8.2	REACH chronic = 8.2 (acute = 300)
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.18 Trichlorobenzenes

Background parameters and concentrations

Substance	trichlorobenzenes		
CAS #		12002-48-1	
M.W. (g/mol)		181	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.1	4.05	EU dossier (TCB)
Koc(l/kg TS)	2089	1400	EU dossier (TCB)
K _D (l/kg TS)	21	14	0.01 Koc
Henry (-)	0.0039	0.0039	
BCF fish (l/kg w.w.)	1200	1140	(Naturvårdsverket, 2005); EU dossier (TCB) used 2000
BCF stem	5.92	6.04	
BCF root	36.4	40.5	
MTDI (mg/kg/d)	0.0077	0.008	RIVM (2001) = 0.008; EU dossier (trichlorobenzenes) = 0.060
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	0.008	0.008	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.08	0.08	
Background			
Freshwater (µg/L)	-	0	
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	0.017 (1,2,4-trichloro)	0.017 (1,2,4-trichloro)	

4.19 1,2,4,5-Tetrachlorobenzene

Background parameters and concentrations

Substance	1,2,4,5-tetrachlorobenzene		
CAS # M.W. (g/mol)		95-94-3 216	<i>not revised due to lack of data</i>
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.6		
Koc(l/kg TS)	5888		
KD(l/kg TS)	59		
Henry (-)	0.54		
BCF fish (l/kg w.w.)	4830		
BCF stem	6.22		
BCF root	126.4		
MTDI (mg/kg/d)	0.0003		
MTDI cancer (mg/kg/d)	-		
RfC (mg/m ³)	-		
RfC cancer (mg/m ³)	-		
Skin contact: f _{du}	0.1		
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.20 Pentachlorobenzene

Background parameters and concentrations

Substance	pentachlorobenzen		
	e		
CAS #		608-93-5	
M.W. (g/mol)		250	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.2	5.2	5.03 - 5.2 EU dossier (pentachlorobenzene)
Koc(l/kg TS)	8318	40000	variable (25120 - 129000), EU dossier (pentachlorobenzene)
KD(l/kg TS)	83	400	0.01 Koc
Henry (-)	0.15	0.15	
BCF fish (l/kg w.w.)	260000	5300	variable (3000 - 20000), "intermediate" value used in EU dossier (pentachlorobenzene)
BCF stem	5.15	5.06	
BCF root	289.8	306	
MTDI (mg/kg/d)	0.0008	0.0005	EU dossier (pentachlorobenzene) = 0.0005, 0.0008
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	0	
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	-	-	

4.21 Hexachlorobenzene

Background parameters and concentrations

Substance	hexachlorobenzene		
CAS #		118-74-1	
M.W. (g/mol)		285	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.7	5.7	EPISuite
Koc(l/kg TS)	11482	130000	EU dossier (HCB)
K_D(l/kg TS)	115	1300	0.01 Koc
Henry (-)	0.0064	0.0064	
BCF fish (l/kg w.w.)	30000	42000	EU dossier (HCB) as BAF
BCF stem	4.05	3.36	
BCF root	522.1	740	
MTDI (mg/kg/d)	0.00003	0.00016	RIVM (2001) CR _{oral} = 0.00016
MTDI cancer (mg/kg/d)	0.000033	0.000033	
RfC (mg/m³)	0.003	0.003	
RfC cancer (mg/m³)	0.00075	0.00075	
Skin contact: f_{du}	0.13	0.13	
Background			
Freshwater (µg/L)	-	0	
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	0.0004-0.006	0.0004-0.006	

4.22 Dichloromethane

Background parameters and concentrations

Substance	dichloromethane		
CAS #	75-09-2		
M.W. (g/mol)	85		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	1.25	1.3	EU dossier (dichloromethane)
Koc(l/kg TS)	16.6	8.8	EU dossier (dichloromethane)
K_D(l/kg TS)	0.17	0.088	0.01 Koc
Henry (-)	0.0861	0.11	EU dossier (dichloromethane)
BCF fish (l/kg w.w.)	5	2.5	calculated EU-TGD (2011)
BCF stem	1.06	0.69	
BCF root	1.65	1.12	
MTDI (mg/kg/d)	0.006	0.06	RIVM (2001) = 0.06; REACH chronic = 0.06
MTDI cancer (mg/kg/d)	0.0013	0.0013	
RfC (mg/m³)	0.45	88.3	REACH chronic = 88.3 (acute = 353)
RfC cancer (mg/m³)	0.05	0.05	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.23 Trichloromethane

Background parameters and concentrations

Substance	trichloromethane		
CAS #		67-66-3	
M.W. (g/mol)		119	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	1.97	1.97	EU dossier (trichloromethane)
Koc(l/kg TS)	46	185	EU dossier (trichloromethane)
K_D(l/kg TS)	0.46	1.9	0.01 Koc
Henry (-)	0.11	0.11	EU dossier (trichloromethane)
BCF fish (l/kg w.w.)	13	13	EU dossier (trichloromethane)
BCF stem	1.13	1.15	
BCF root	1.78	1.81	
MTDI (mg/kg/d)	0.013	0.03	RIVM (2001) = 0.03
MTDI cancer (mg/kg/d)	0.000164	0.000164	
RfC (mg/m³)	0.045	0.18	REACH = 0.18
RfC cancer (mg/m³)	0.024	0.024	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.24 Trichloroethene

Background parameters and concentrations

Substance	trichloroethene		
CAS #		79-01-6	
M.W. (g/mol)		131	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.6	2.5	REACH Reliability 2 (20 °C)
Koc(l/kg TS)	115	141	REACH Reliability 2
K_D(l/kg TS)	1.15	1.4	0.01 Koc
Henry (-)	0.28	0.42	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	17	28	calculated EU-TGD (2011)
BCF stem	1.74	1.92	
BCF root	3.08	3.50	
MTDI (mg/kg/d)	0.0015	0.05	RIVM (2001) = 0.05
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.023	0.023	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.25 Tetrachloromethane

Background parameters and concentrations

Substance	tetrachloro-methane		
CAS # M.W. (g/mol)		56-23-5 154	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.7	2.83	REACH Reliability 2 (25 °C)
Koc(l/kg TS)	174	84.1	REACH Reliability 2 (median 1.69- 2.16)
KD(l/kg TS)	1.7	0.8	0.01 Koc
Henry (-)	1.25	1.21	REACH Reliability 2
BCF fish (l/kg w.w.)	17	51	calculated EU-TGD (2011)
BCF stem	-	2.58	
BCF root	-	5.38	
MTDI (mg/kg/d)	0.007	0.004	RIVM (2001) = 0.004
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	0.0061	0.107	REACH = 0.107
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.1	0.00046	REACH Reliability 4
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.26 Tetrachloroethene

Background parameters and concentrations

Substance	tetrachloroethene		
CAS #		127-18-4	
M.W. (g/mol)		166	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.4	2.53	REACH Reliability 2 (23 °C)
Koc(l/kg TS)	263	141	REACH Reliability 3
K_D(l/kg TS)	2.6	1.4	0.01 Koc
Henry (-)	0.93	0.87	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	77.1	28	calculated EU-TGD (2011)
BCF stem	1.96	1.92	
BCF root	3.61	3.51	
MTDI (mg/kg/d)	0.014	0.016	RIVM (2001) = 0.016; REACH chronic = 1.3
MTDI cancer (mg/kg/d)	0.0002	0.0002	
RfC (mg/m³)	0.25	34.5	REACH chronic= 34.5 (acute = 138)
RfC cancer (mg/m³)	0.0055	0.0055	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.27 1,2-dichloroethane

Background parameters and concentrations

Substance	1,2-dichloroethane		
CAS #		540-59-0	
M.W. (g/mol)		97	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	1.477	1.45	EU dossier (1,2-DCE)
Koc(l/kg TS)	30.9	116	EU dossier (1,2-DCE)
K_D(l/kg TS)	0.3	1.2	0.01 Koc
Henry (-)	0.03	0.045	EU dossier (1,2-DCE)
BCF fish (l/kg w.w.)	3	2	EU dossier (1,2-DCE)
BCF stem	0.79	0.77	
BCF root	1.23	1.21	
MTDI (mg/kg/d)	-	0.014	RIVM (2001) CR _{oral} = 0.014
MTDI cancer (mg/kg/d)	0.00012	0.00012	
RfC (mg/m³)	-	0.0029	REACH = 0.0029
RfC cancer (mg/m³)	0.0036	0.0036	
Skin contact: f_{du}	0.1	1	REACH Reliability 2 exp, Values >100%, used 100%
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.28 1,2-dibromoethane

Background parameters and concentrations

Substance	1,2-dibromoethane		
CAS #		106-93-4	
M.W. (g/mol)		188	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	1.96	1.96	REACH Reliability 2
Koc(l/kg TS)	43.8	40.7	REACH Reliability 2 (median 1.11;1.61;1.65)
K_D(l/kg TS)	0.44	0.41	0.01 Koc
Henry (-)	0.03	0.03	REACH Reliability 2 (estimated median)
BCF fish (l/kg w.w.)	9.1	9.2	calculated EU-TGD (2011)
BCF stem	1.13	1.14	
BCF root	1.79	1.80	
MTDI (mg/kg/d)	-	-	
MTDI cancer (mg/kg/d)	0.000035	0.000035	
RfC (mg/m³)	-	1.15	REACH chronic = 1.15 (acute = 2)
RfC cancer (mg/m³)	0.00005	0.00005	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.29 1,1,1-trichloroethane

Background parameters and concentrations

Substance	1,1,1-trichloroethane		
CAS # M.W. (g/mol)		71-55-6 133	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.49	2.5	REACH Reliability 2
Koc(l/kg TS)	110	110	
KD(l/kg TS)	1.1	1.1	0.01 Koc
Henry (-)	0.71	0.0007	REACH (reliability not given)
BCF fish (l/kg w.w.)	9	27	calculated EU-TGD (2011)
BCF stem	1.72	1.86	
BCF root	3.03	3.36	
MTDI (mg/kg/d)	0.58	0.58	
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.8	0.8	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.30 1,1,2-trichloroethane

Background parameters and concentrations

Substance	1,1,2-trichloro-ethane		
CAS # M.W. (g/mol)	79-00-5 133		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	1.89	2.27	REACH Reliability 2 (20 °C, median used 2.05-2.49)
Koc(l/kg TS)	80	80	
K _D (l/kg TS)	0.8	0.8	0.01 Koc
Henry (-)	0.9	0.04	REACH Reliability 2 (estimated, median used)
BCF fish (l/kg w.w.)	-	17	calculated EU-TGD (2011)
BCF stem	-	1.49	
BCF root	-	2.51	
MTDI (mg/kg/d)	0.004	0.004	
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	-	-	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.31 Phenol

Background parameters and concentrations

Substance	phenol		
CAS #		108-95-2	
M.W. (g/mol)		94	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	1.47	1.47	REACH Reliability 2 (30 °C)
Koc(l/kg TS)	30	30	
K_D(l/kg TS)	0.3	0.3	0.01 Koc
Henry (-)	0.000000218	0.000013	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	17.5	3.5	calculated EU-TGD (2011)
BCF stem	-	0.79	
BCF root	-	1.23	
MTDI (mg/kg/d)	0.04	0.04	RIVM (2001) = 0.04; REACH chronic value = 0.4
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	1.32	REACH value = 1.32
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.26	0.8	REACH Reliability 2 exp
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.32 Sum mono-tetrachlorophenols

Background parameters and concentrations

Substance	sum mon-tetrachlorophenols		
CAS # M.W. (g/mol)	n.a. n.a.		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.7	3.7	
Koc(l/kg TS)	30	30	
KD(l/kg TS)	0.3	0.3	0.01 Koc
Henry (-)	0.00004	0.00004	
BCF fish (l/kg w.w.)	-	279	calculated EU-TGD (2011)
BCF stem	-	5.20	
BCF root	-	22.2	
MTDI (mg/kg/d)	0.0067	0.003	RIVM (2001) mono, di, tri and tetrachlorophenols are individually = 0.003
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.26	0.26	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

n.a. = not applicable

4.33 Pentachlorophenol

Background parameters and concentrations

Substance	pentachlorophenol		
CAS #		87-86-5	
M.W. (g/mol)		266	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.1	3	at pH 7 (log Pow can range from 5 – 1 in soil, depending on the pH)
Koc(l/kg TS)	1585	3400	706 - 53000 variable with pH - EU dossier (pentachlorophenol)
K_D(l/kg TS)	16	34	0.01 Koc
Henry (-)	0.000226	0.000226	
BCF fish (l/kg w.w.)	1250	770	770 used as worst case (EU dossier pentachlorophenol), values range from 91 - 1000 (variable)
BCF stem	5.42	3.04	
BCF root	247.3	247	estimated value = 7.0
MTDI (mg/kg/d)	0.003	0.003	RIVM (2001); EU dossier (pentachlorophenol) = 30 = 0.003
MTDI cancer (mg/kg/d)	0.000083	0.000083	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.0000075	0.0000075	
Skin contact: f_{du}	0.11	0.11	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	<0.005	<0.005	

4.34 Naphthalene

Background parameters and concentrations

Substance	naphthalene		
CAS #	91-20-3		
M.W. (g/mol)	128		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.3	3.3	EU dossier (naphthalene)
Koc(l/kg TS)	995	1349	Karickhoff et al., (1979)
K_D(l/kg TS)	10	13	0.01 Koc
Henry (-)	0.0117	0.0117	
BCF fish (l/kg w.w.)	229	515	EU dossier (naphthalene)
BCF stem	4.14	3.95	
BCF root	12.5	11.3	
MTDI (mg/kg/d)	0.04	0.04	RIVM (2001) = 0.04
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.003	0.003	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.1	0.83	REACH Reliability 2 exp, median used (0,876; 0,78)
Background			
Freshwater (µg/L)	-	0.000661	assumed same as coastal water
Coastal water (µg/L)	-	0.000661	OSPAR (2006) Max North, North Sea
Sediment (mg/kg)	-	0.002	OSPAR (2006)
Soil (mg/kg)	m.d	0.011	Nam et al. (2008)

4.35 Acenaphthylene

Background parameters and concentrations

Substance	acenaphthylene		
CAS #		208-96-8	
M.W. (g/mol)		152	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.9	3.55	RIVM (2012)
Koc(l/kg TS)	2951	2570	EU RAR (coal tar pitch) – after Karickhoff et al., (1979)
K_D(l/kg TS)	30	26	0.01 Koc
Henry (-)	0.029	0.029	
BCF fish (l/kg w.w.)	-	509	RIVM (2009) - Cyprinus carpio (fish), 5% norm
BCF stem	-	4.74	
BCF root	-	17.2	
MTDI (mg/kg/d)	0.04	0.05	RIVM (2001) = 0.05
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.18	0.18	
Background			
Freshwater (µg/L)	-	0.00001	(OSPAR 2006 N North Sea)
Coastal water (µg/L)	-	0.00001	(OSPAR 2006)
Sediment (mg/kg)	-	0.0016	(OSPAR 2006 N North Sea)
Soil (mg/kg)	-	-	

4.36 Acenaphthene

Background parameters and concentrations

Substance	acenaphthene		
CAS #		83-32-9	
M.W. (g/mol)		154	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.9	3.92	RIVM (2012)
Koc(l/kg TS)	3388	5129	EU RAR (coal tar pitch)
K_D(l/kg TS)	34	51	0.01 Koc
Henry (-)	0.011	0.011	
BCF fish (l/kg w.w.)	-	1000	RIVM (2009) - Cyprinus carpio (fish), 5% norm
BCF stem	-	5.77	
BCF root	-	32.3	
MTDI (mg/kg/d)	0.04	0.5	RIVM (2001) = 0.5
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000034	(OSPAR 2006)
Coastal water (µg/L)	-	0.000034	(OSPAR 2006)
Sediment (mg/kg)	-	0.0024	(OSPAR 2006), TA-2803 = 4.8
Soil (mg/kg)	-	0.0032	Nam et al. (2008)

4.37 Phenanthrene

Background parameters and concentrations

Substance	phenanthrene		
CAS #		85-01-8	
M.W. (g/mol)		178	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.47	4.502	RIVM (2012)
Koc(l/kg TS)	16982	37154	EU RAR (coal tar pitch)
K _D (l/kg TS)	170	372	0.01 Koc
Henry (-)	0.00135	0.00135	
BCF fish (l/kg w.w.)	1476	4751	RIVM (2009) - 4751 fish, 14893 crustaceans
BCF stem	-	6.39	
BCF root	-	89.2	
MTDI (mg/kg/d)	0.04	0.04	RIVM (2001) = 0.04
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.18	0.18	
Background			
Freshwater (µg/L)	-	0.000254	(OSPAR 2006)
Coastal water (µg/L)	-	0.000254	(OSPAR 2006)
Sediment (mg/kg)	-	0.0068	(OSPAR 2006)
Soil (mg/kg)	-	0.04	Nam et al. (2008)

4.38 Anthracene

Background parameters and concentrations

Substance	anthracene		
CAS #		120-12-7	
M.W. (g/mol)		178	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.45	4.68	EU dossier (anthracene)
Koc(l/kg TS)	19953	29512	EU dossier (anthracene) (uses Karickhoff et al., 1979 log Koc = log Kow - 0.21)
Kd(l/kg TS)	200	295	0.01 Koc
Henry (-)	0.0009	0.0021	REACH Reliability 4
BCF fish (l/kg w.w.)	1409	3042	EU dossier (anthracene)
BCF stem	-	6.25	
BCF root	-	122	
MTDI (mg/kg/d)	0.04	0.04	RIVM (2001) = 0.04
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.004	assumed same as coastal water
Coastal water (µg/L)	-	0.004	OSPAR (2006) Max
Sediment (mg/kg)	-	0.0012	OSPAR (2006)
Soil (mg/kg)	-	0.0034	Nam et al. (2008)

4.39 Fluorene

Background parameters and concentrations

Substance	fluorene		
CAS #		86-73-7	
M.W. (g/mol)		166	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.21005085	4.18	RIVM (2012)
Koc(l/kg TS)	5886	10233	EU RAR (2008c)
K _D (l/kg TS)	59	102	0.01 Koc
Henry (-)	0.00619	0.00619	
BCF fish (l/kg w.w.)	-	1658	RIVM (2009) - <i>Pimephales promelas</i> (fish), 5% norm
BCF stem	-	6.24	
BCF root	-	50.8	
MTDI (mg/kg/d)	0.04	0.04	RIVM (2001) = 0.04
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.00019	(OSPAR 2006)
Coastal water (µg/L)	-	0.00019	(OSPAR 2006)
Sediment (mg/kg)	-	0.0068	(OSPAR 2006 N North Sea)
Soil (mg/kg)	-	0.0068	Nam et al. (2008)

4.40 Fluoranthene

Background parameters and concentrations

Substance	fluoranthene		
CAS #		206-44-0	
M.W. (g/mol)		202	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.120573931	5.2	EU dossier (fluoranthene)
Koc(l/kg TS)	141336	97724	EU dossier (fluoranthene) (uses Karickhoff et al., 1979 log Koc = log Kow - 0.21)
Kd(l/kg TS)	1514	977	0.01 Koc
Henry (-)	0.00163	0.00163	
BCF fish (l/kg w.w.)	13200	4800	EU dossier (fluoranthene)
BCF stem	5.3	5.06	
BCF root	266	306	
MTDI (mg/kg/d)	0.0125	0.05	RIVM (2001) = 0.05
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.000012	0.000012	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.00029	assumed same as coastal water
Coastal water (µg/L)	-	0.00029	OSPAR (2006) Max
Sediment (mg/kg)	-	0.008	OSPAR (2006)
Soil (mg/kg)	-	0.014	Nam et al. (2008)

4.41 Pyrene

Background parameters and concentrations

Substance	pyrene		
CAS #		129-00-0	
M.W. (g/mol)		202	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.11058971	4.96	RIVM (2012)
Koc(l/kg TS)	67608	58884	EU RAR (2008c)
K _D (l/kg TS)	676	589	0.01 Koc
Henry (-)	0.0000749	0.0000749	RIVM (2009) - 1474 fish, 44500 mollusks, 88157 crustaceans (benthic fauna recommended for large PAHs, see Directive 2013/39/EU)
BCF fish (l/kg w.w.)	-	88157	
BCF stem	-	5.73	
BCF root	-	200	
MTDI (mg/kg/d)	0.03	0.5	RIVM (2001) = 0.5
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000053	(OSPAR 2006)
Coastal water (µg/L)	-	0.000053	(OSPAR 2006)
Sediment (mg/kg)	-	0.0052	(OSPAR 2006)
Soil (mg/kg)	-	0.013	Nam et al. (2008)

4.42 Benzo(a)anthracene

Background parameters and concentrations

Substance	benzo(a)-anthracene		
CAS # M.W. (g/mol)		56-55-3 228	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.54	5.91	RIVM (2012)
Koc(l/kg TS)	616595	501187	RIVM (2012)
K _D (l/kg TS)	6172	5012	0.01 Koc
Henry (-)	0.0000017	0.0000017	
BCF fish (l/kg w.w.)	17337	33457	RIVM (2009) - 260 fish, 33457 crustaceans (benthic fauna recommended for large PAHs, see Directive 2013/39/EU)
BCF stem	-	2.66	
BCF root	-	1074	
MTDI (mg/kg/d)	0.005	0.005	RIVM (2001) = 0.005
MTDI cancer (mg/kg/d)	0.00023	0.00023	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	0.0000077	0.0000077	
Skin contact: f _{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000006	(OSPAR 2006)
Coastal water (µg/L)	-	0.000006	(OSPAR 2006)
Sediment (mg/kg)	-	0.0036	(OSPAR 2006)
Soil (mg/kg)	-	0.0045	Nam et al. (2008)

4.43 Chrysene

Background parameters and concentrations

Substance	chrysene		
CAS #	218-01-9		
M.W. (g/mol)	228		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.81	5.81	RIVM (2012)
Koc(l/kg TS)	524807	398107	RIVM (2012)
K_D(l/kg TS)	5253	3981	0.01 Koc
Henry (-)	0.0000047	0.0000047	
BCF fish (l/kg w.w.)	32283	6088	RIVM (2009) - crustaceans
BCF stem	-	2.99	
BCF root	-	900	
MTDI (mg/kg/d)	-	0.05	RIVM (2001) = 0.05
MTDI cancer (mg/kg/d)	0.0023	0.0023	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.0000012	0.0000012	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000056	(OSPAR 2006)
Coastal water (µg/L)	-	0.000056	(OSPAR 2006)
Sediment (mg/kg)	-	0.0044	(OSPAR 2006)
Soil (mg/kg)	-	0.014	Nam et al. (2008)

4.44 Benzo(b)fluoranthene

Background parameters and concentrations

Substance	benzo(b)-fluoranthene		
CAS # M.W. (g/mol)	205-99-2 252		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.78	5.78	EU dossier (5,6-ring PAHs)
Koc(l/kg TS)	218776	831864	EU dossier (5,6-ring PAHs) (uses Karickhoff et al., 1979 log Koc = log Kow - 0.21, but the estimated Kow of 2.12)
KD(l/kg TS)	2188	8319	0.01 Koc
Henry (-)	0.0000028	0.0000028	EU dossier (5,6-ring PAHs): 135 (fish) 11138 (crustaceans) 57981 (mollusks), WFD recommends crustaceans and mollusks as basis
BCF fish (l/kg w.w.)	50000	11138	
BCF stem	-	3.09	
BCF root	-	853	
MTDI (mg/kg/d)	0.005	0.005	RIVM (2001) = 0.005
MTDI cancer (mg/kg/d)	0.00023	0.00023	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.00000083	0.00000083	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000017	assumed same as coastal water
Coastal water (µg/L)	-	0.000017	OSPAR (2006) Max
Sediment (mg/kg)	-	0.0916	OSPAR (2006) - N North Sea benzo(b + k)fluoranthene divided by two
Soil (mg/kg)	-	0.016	Nam et al. (2008)

4.45 Benzo(k)fluoranthene

Background parameters and concentrations

Substance	benzo(k)-fluoranthene		
CAS # M.W. (g/mol)	207-08-9 252		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.11	6.11	EU dossier (5,6-ring PAHs)
Koc(l/kg TS)	1737801	794328	EU dossier (5,6-ring PAHs) (uses Karickhoff et al., 1979 log Koc = log Kow - 0.21)
K_D(l/kg TS)	17395	7943	0.01 Koc
Henry (-)	0.0000028	0.0000028	
BCF fish (l/kg w.w.)	50000	11138	EU dossier (5,6-ring PAHs), 135 (fish) 11138 (crustaceans) 57981 (mollusks), WFD recommends crustaceans and mollusks as basis
BCF stem	-	2.06	
BCF root	-	1531	
MTDI (mg/kg/d)	-	0.005	RIVM (2001) = 0.005
MTDI cancer (mg/kg/d)	0.00023	0.00023	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.0000012	0.0000012	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000017	assumed same as coastal water
Coastal water (µg/L)	-	0.000017	OSPAR (2006) assumed same as Benzo(b)fluoranthene
Sediment (mg/kg)	-	0.0916	OSPAR (2006) - N North Sea benzo(b + k)fluoranthene divided by two
Soil (mg/kg)	-	0.0031	Nam et al. (2008)

4.46 Benzo(a)pyrene

Background parameters and concentrations

Substance	benzo(a)pyrene		
CAS #		50-32-8	
M.W. (g/mol)		252	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.4	6.11	EU dossier (5,6-ring PAHs)
Koc(l/kg TS)	660693	831764	EU dossier (5,6-ring PAHs): (uses Karickhoff et al., 1979 , but used log Koc = log Kow - 0.19 instead of log Koc = log Kow - 0.21)
K_D(l/kg TS)	-	8318	0.01 Koc
Henry (-)	0.000034	0.000034	
BCF fish (l/kg w.w.)	28200	11138	EU dossier (5,6-ring PAHs): 135 (fish) 11138 (crustaceans) 57981 (mollusks), WFD recommends crustaceans and mollusks as basis
BCF stem	2.01	2.06	
BCF root	1584	1531	
MTDI (mg/kg/d)	0.00001	0.0005	RIVM (2001) = 0.0005
MTDI cancer (mg/kg/d)	0.00001	0.00001	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.00000011	0.00000011	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0.000005	assumed same as coastal water
Coastal water (µg/L)	-	0.000005	OSPAR (2006) Max
Sediment (mg/kg)	-	0.006	OSPAR (2006)
Soil (mg/kg)	<0.01-0.16	0.0053	Nam et al. (2008)

4.47 Indeno(1,2,3-cd)pyrene

Background parameters and concentrations

Substance	indeno(1,2,3-cd)-pyrene		
CAS # M.W. (g/mol)		193-39-5 276	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.87	6.7	EU dossier (5,6-ring PAHs)
Koc(l/kg TS)	1047129	2344229	EU dossier (5,6-ring PAHs) (uses Karickhoff et al., 1979 , but used log Koc = log Kow - 0.33 instead of log Koc = log Kow - 0.21)
KD(l/kg TS)	10482	23442	0.01 Koc
Henry (-)	0.00000117	0.00000117	
BCF fish (l/kg w.w.)	50000	11138	EU dossier (5,6-ring PAHs): 135 (fish) 11138 (crustaceans) 57981 (mollusks), WFD recommends crustaceans and mollusks as basis
BCF stem	-	0.80	
BCF root	-	4356	
MTDI (mg/kg/d)	0.005	0.005	RIVM (2001) = 0.005
MTDI cancer (mg/kg/d)	0.00023	0.00023	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	0.0000005	0.0000005	
Skin contact: f_{du}	0.18	0.18	
Background			
Freshwater (µg/L)	-	0.000017	assumed same as coastal water
Coastal water (µg/L)	-	0.000017	OSPAR (2006) Max
Sediment (mg/kg)	-	0.02	OSPAR (2006)
Soil (mg/kg)	-	-	

4.48 Dibenzo(a,h)anthracene

Background parameters and concentrations

Substance	dibenzo(a,h)-anthracene		
CAS # M.W. (g/mol)		53-70-3 278	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	7.11	6.55	RIVM (2012)
Koc(l/kg TS)	1380384	1949845	RIVM (2012)
KD(l/kg TS)	18804	19498	0.01 Koc
Henry (-)	0.000038	0.000038	
BCF fish (l/kg w.w.)	50000	50119	RIVM (2009) - crustaceans
BCF stem	-	1.05	
BCF root	-	3339	
MTDI (mg/kg/d)	-	0.0005	RIVM (2001) = 0.0005
MTDI cancer (mg/kg/d)	0.000023	0.000023	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	0.000000023	0.000000023	
Skin contact: f _{du}	0.09	0.09	
Background			
Freshwater (µg/L)	-	0.000001	(OSPAR 2006) max "<0.000001 µg/L)
Coastal water (µg/L)	-	0.000001	(OSPAR 2006) max "<0.000001 µg/L)
Sediment (mg/kg)	-	0.012	(OSPAR 2006 N North Sea)
Soil (mg/kg)	-	0.0012	Nam et al. (2008)

4.49 Benzo(g,h,i)perylene

Background parameters and concentrations

Substance	benzo(g,h,i)perylene		
CAS #		191-24-2	
M.W. (g/mol)		276	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.22	6.63	EU dossier (5,6-ring PAHs)
Koc(l/kg TS)	2691535	1023293	EU dossier (5,6-ring PAHs) (uses Karickhoff et al., 1979 , but used log Koc = log Kow - 0.62 instead of log Koc = log Kow - 0.21)
K_D(l/kg TS)	26942	10233	0.01 Koc
Henry (-)	0.000004	0.000004	
BCF fish (l/kg w.w.)	50000	11138	EU dossier (5,6-ring PAHs): 135 (fish) 11138 (crustaceans) 57981 (mollusks), WFD recommends crustaceans and mollusks as basis
BCF stem	-	0.91	
BCF root	-	3848	
MTDI (mg/kg/d)	0.03	0.03	RIVM (2001) = 0.03
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.18	0.18	
Background			
Freshwater (µg/L)	-	0.000011	assumed same as coastal water
Coastal water (µg/L)	-	0.000011	OSPAR (2006) Max
Sediment (mg/kg)	-	0.018	OSPAR (2006)
Soil (mg/kg)	-	0.0093	Nam et al. (2008)

4.50 PAH total

Each of the PAHs has unique properties. However, they are normally present in the environment as mixtures. Studies on PAH mixture composition found that generally the concentration of 3 and 4 ring PAHs correlated the best with concentrations of all other PAHs, across diverse types of sediments (Arp et al. 2011). Pyrene was chosen as a result of its good correlation to the PAH-16 concentration. To demonstrate that this also applies to soils, a data base of PAHs in diverse contaminated soils from Europe, originating from Arp et al. (2014) was analysed and showed the following correlation:

$$C_{\text{soil,PAH-16}} = 5.71 \pm 0.23 (C_{\text{soil,pyrene}}) \quad (r^2 = 0.95)$$

Compound specific parameters for PAH-16 are therefore set identical to pyrene (chapter 4.50). However, human health is controlled by the most critical parameter which is normally benzo(a)pyrene.

Background parameters and concentrations

Substance	PAH-16		
CAS # M.W. (g/mol)			
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.4	4.96	see Pyrene
Koc(l/kg TS)	66093	58884	see Pyrene
K_D(l/kg TS)	6607	589	0.01 Koc
Henry (-)	0.02	0.0000749	see Pyrene
BCF fish (l/kg w.w.)	28200	88157	see Pyrene
BCF stem	2.01	5.73	see Pyrene
BCF root	1584	200	see Pyrene
MTDI (mg/kg/d)	See BaP		BaP determines human health
MTDI cancer (mg/kg/d)	See BaP		BaP determines human health
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	See BaP		BaP determines human health
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	0,0056	assumed same as coastal water
Coastal water (µg/L)	-	0,0056	OSPAR (2006) Max North, North Sea
Sediment (mg/kg)	-	0,281	OSPAR (2006)
Soil (mg/kg)	-	0,145	PAH-14, Nam et al, (2008)

4.51 Benzene

Background parameters and concentrations

Substance	benzene		
CAS #		71-43-2	
M.W. (g/mol)		78	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.1	2.13	EU dossier (benzene)
Koc(l/kg TS)	74	134	EU dossier (benzene)
K_D(l/kg TS)	0.7	1.3	0.01 Koc
Henry (-)	0.159	0.159	
BCF fish (l/kg w.w.)	10.9	13	EU dossier (benzene)
BCF stem	1.32	1.31	
BCF root	2.15	2.14	
MTDI (mg/kg/d)	-	0.007	RIVM (2001) = 0.007
MTDI cancer (mg/kg/d)	0.00033	0.00033	
RfC (mg/m³)	0.05	0.05	
RfC cancer (mg/m³)	0.0012	0.0012	
Skin contact: f_{du}	0.08	0.015	REACH Reliability 2 (QSAR)
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	<0.1	<0.1	

4.52 Toluene

Background parameters and concentrations

Substance	toluene		
CAS #		108-88-3	
M.W. (g/mol)		92	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.8	2.73	REACH Reliability 2 (20 °C)
Koc(l/kg TS)	250	63.8	REACH Reliability 4 (median 1.53-2.08)
K_D(l/kg TS)	2.5	0.64	0.01 Koc
Henry (-)	0.27	0.27	
BCF fish (l/kg w.w.)	39	42	calculated EU-TGD (2011)
BCF stem	2.2	2.34	
BCF root	4.24	4.64	
MTDI (mg/kg/d)	0.22	0.223	RIVM (2001) = 0.223; REACH chronic = 8.13
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.26	56.5	REACH chronic = 56.5 (acute = 226)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.12	0.036	REACH Reliability 2 (Q)Sar
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	0.32	0.32	

4.53 Ethylbenzene

Background parameters and concentrations

Substance	ethylbenzene		
CAS #		100-41-4	
M.W. (g/mol)		106	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.8	3.6	REACH Reliability 1 (20 °C)
Koc(l/kg TS)	250	250	
K_D(l/kg TS)	2.5	2.5	0.01 Koc
Henry (-)	0.27	0.33	REACH Reliability 2
BCF fish (l/kg w.w.)	86	229	calculated EU-TGD (2011)
BCF stem	3.4	4.90	
BCF root	8.48	18.7	
MTDI (mg/kg/d)	0.1	0.1	RIVM (2001) = 0.1; REACH chronic = 1.6
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	1	15	REACH chronic = 15 (worker = 77)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	<0.1	<0.1	

4.54 Xylene

Background parameters and concentrations

Substance	xylene		
CAS #		1330-20-7	
M.W. (g/mol)		106	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	2.8	3.2	REACH Reliability 2 (20 °C)
Koc(l/kg TS)	250	250	
K_D(l/kg TS)	2.5	2.5	0.01 Koc
Henry (-)	0.27	0.26	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	105	105	calculated EU-TGD (2011)
BCF stem	3.37	3.64	
BCF root	8.34	9.61	
MTDI (mg/kg/d)	0.2	0.15	RIVM (2001) = 0.15; REACH chronic = 1.6
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	0.87	14.8	REACH chronic = 14.8 (acute = 174)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.12	0.118	REACH Reliability 2 (Q)Sar, median used (0.139; 0.118; 0.109)
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	<0.1	<0.1	

4.55 Aliphatics C5-C6

Background parameters and concentrations

Substance	aliphatics C5-C6		
CAS #		n.a.	
M.W. (g/mol)		n.a.	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.278754	3.3	
Koc(l/kg TS)	800	800	
K_D(l/kg TS)	8	8	0.01 Koc
Henry (-)	47	47	
BCF fish (l/kg w.w.)	190	122	calculated EU-TGD (2011)
BCF stem	3.88	3.88	
BCF root	10.93	10.9	
MTDI (mg/kg/d)	5	2	RIVM (2001): C5-C8 = 2
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	18.4	18.4	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	1	1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.56 Aliphatics > C6-C8

Background parameters and concentrations

Substance	aliphatics > C6-C8		
CAS # M.W. (g/mol)		n.a. n.a.	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.0	4.0	
Koc(l/kg TS)	4000	4000	
K_D(l/kg TS)	40	40	0.01 Koc
Henry (-)	50	50	
BCF fish (l/kg w.w.)	970	488	calculated EU-TGD (2011)
BCF stem	5.92	5.92	
BCF root	36.28	36.3	
MTDI (mg/kg/d)	5	2	RIVM (2001) - C5-C8 = 2
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	18.4	18.4	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	1	1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.57 Aliphatics > C8-C10

Background parameters and concentrations

Substance	aliphatics > C8-C10		
CAS # M.W. (g/mol)	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.886490725	4.9	
Koc(l/kg TS)	32000	32000	
K_D(l/kg TS)	320	320	0.01 Koc
Henry (-)	55	55	
BCF fish (l/kg w.w.)	7700	2841	calculated EU-TGD (2011)
BCF stem	5.9	5.90	
BCF root	175.64	176	
MTDI (mg/kg/d)	0.1	0.1	RIVM (2001): C18-C16 = 0.1
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	1	1	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.5	0.5	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.58 Sum aliphatics > C5-C10

Background parameters and concentrations

Substance	sum aliphatics > C5-C10		
	CAS #	n.a.	
M.W. (g/mol)	n.a.		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.9	3.9	
Koc(l/kg TS)	-	-	
K _D (l/kg TS)	-	-	
Henry (-)	34	34	
BCF fish (l/kg w.w.)	-	412	calculated EU-TGD (2011)
BCF stem	-	5.72	
BCF root	-	31.2	
MTDI (mg/kg/d)	0.1	0.1	
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	1	1	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.59 Aliphatics > C10-C12

Background parameters and concentrations

Substance	aliphatics > C10-C12		
	CAS #	n.a.	
M.W. (g/mol)	n.a.		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.77815125	5.8	
Koc(l/kg TS)	250000	250000	
K _D (l/kg TS)	2500	2500	0.01 Koc
Henry (-)	60	60	
BCF fish (l/kg w.w.)	60000	16272	calculated EU-TGD (2011)
BCF stem	3.09	3.09	
BCF root	850.35	850	
MTDI (mg/kg/d)	0.1	0.1	RIVM (2001): C18-C16 = 0.1
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	1	1	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.5	0.5	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.60 Aliphatics > C12-C35

Background parameters and concentrations

Substance	aliphatics > C12-C35		
CAS # M.W. (g/mol)	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.3	6.3	
Koc(l/kg TS)	1.0E+09	1.0E+09	
K _D (l/kg TS)	1.0E+07	1.0E+07	0.01 Koc
Henry (-)	87	87	
BCF fish (l/kg w.w.)	200000000	40179	calculated EU-TGD (2011)
BCF stem	0.0004	1.57	
BCF root	438322	2144	
MTDI (mg/kg/d)	2	2	
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	1	1	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.1	0.1	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.61 MTBE

Background parameters and concentrations

Substance	MTBE		
CAS #		1634-04-4	
M.W. (g/mol)		88	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	0.9	1.23	REACH Reliability 1
Koc(l/kg TS)	6	6	
K_D(l/kg TS)	0.06	0.06	0.01 Koc
Henry (-)	0.024	0.022	REACH Reliability 2
BCF fish (l/kg w.w.)	2	2	calculated EU-TGD (2011)
BCF stem	0.69	0.66	
BCF root	1.12	1.09	
MTDI (mg/kg/d)	0.1	7.1	REACH chronic = 7.1
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	3	53.6	REACH chronic = 53.6 (acute = 214)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.1	0.002	REACH Reliability 2 (Q)Sar
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.62 Tetraethyl-lead

Background parameters and concentrations

Substance	tetraethyl-lead		
CAS #		78-00-2	
M.W. (g/mol)		323	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.1	4.385	REACH Reliability 2 (20 °C, median used 4.15;4.62)
Koc(l/kg TS)	758	1300	REACH Reliability 2
K_D(l/kg TS)	7.6	13	0.01 Koc
Henry (-)	28	0.19	REACH Reliability 2 minimum value!
BCF fish (l/kg w.w.)	100	1065	calculated EU-TGD (2011)
BCF stem	3.04	6.39	
BCF root	6.99	72.7	
MTDI (mg/kg/d)	1.0E-07	1.0E-07	
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	0.08	REACH chronic = 0.08 (acute = 0.34)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	1	0.065	REACH Reliability 2 exp
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.63 Brominated diphenylethers

Background parameters and concentrations

Substance	brominated diphenylethers		
CAS #	Only Tetra, Penta, Hexa and Heptabromodiphenylether (CAS -numbers 40088-47-9, 32534-81-9, 36483-60-0, 68928-80-3, respectively)		
M.W. (g/mol)	564.7 (pentaBDE); 801.38 (octaBDE)		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	6.285	6.5	EU dossier (BDE): assumes tetra; 5.87 (tetra, lowest measured); 6.57 (penta); 8.35 (lowest measured)
Koc(l/kg TS)	21080	565860	EU dossier (BDE): assumes tetra; 565860 (tetra); 983340 (penta); 1363040 (and larger for octa)
K _D (l/kg TS)	13921	5659	0.01 Koc
Henry (-)	1.2E-06	1.2E-06	
BCF fish (l/kg w.w.)	3245	35000	EU dossier (BDE) highest measured (tetra BDE)
BCF stem	-	1.14	
BCF root	-	3056	
MTDI (mg/kg/d)	0.002	1.4E-07	EU dossier (BDE) = 0.00000014
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	0.067	0.067	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	0.00004 (BDE-99)	-	BDEs do not occur naturally

4.64 PBDE-209

Background parameters and concentrations

Substance	PBDE-209		
CAS #		1163-19-5	
M.W. (g/mol)		959	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	9.9	9.9	REACH = 6.625, which is inconsistent with other BDE; a value between 9.5 - 11 is more consistent (Palm et al. (2002))
Koc(l/kg TS)	33000	5.2E+11	REACH Reliability 2 (estimated)
Kd(l/kg TS)	330	5.2E+09	0.01 Koc
Henry (-)	0.000000045	4.9E-07	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	-	637	calculated EU-TGD (2011)
BCF stem	-	3.3E-05	
BCF root	-	1.27E+06	
MTDI (mg/kg/d)	0.01	20	REACH chronic =20, (acute also = 20)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	70	REACH = 70 (worker = 6)
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.067	0.067	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	0.00051	0.00051	

4.65 HBCDD

Background parameters and concentrations

Substance	HBCDD		
CAS #	This refers to 1,3,5,7,9,11-Hexabromocyclododecane (CAS 25637-99-4), 1,2,5,6,9,10-Hexabromocyclododecane (CAS 3194-55-6), α -Hexabromocyclododecane (CAS 134237-50-6), β -Hexabromocyclododecane (CAS 134237-51-7) and γ -Hexabromocyclododecane (CAS 134237-52-8)		
M.W. (g/mol)	642		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.8	5.62	technical product (EU dossier (HBCDD))
Koc(l/kg TS)	330	45709	technical product (EU dossier (HBCDD))
KD(l/kg TS)	33	457	0.01 Koc
Henry (-)	0.000117	0.000117	
BCF fish (l/kg w.w.)	-	18100	technical product (EU dossier (HBCDD))
BCF stem	-	3.64	
BCF root	-	643	
MTDI (mg/kg/d)	-	0.1	EU dossier (HBCDD) TL value = 0.1; REACH chronic = 0.102
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	0.719	REACH = 0.719
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.067	0.0001	REACH Reliability 1 exp
Background			
Freshwater (µg/L)	-	0 (LOD 0.001)	lowest measured above LOD in TA-2982
Coastal water (µg/L)	-	0 (LOD 0.001)	lowest measured above LOD in TA-2982
Sediment (mg/kg)	-	0	
Soil (mg/kg)	-	-	

4.66 Tetrabromobisphenol A

Background parameters and concentrations

Substance	tetrabromo-bisphenol A		
CAS # M.W. (g/mol)		79-94-7 544	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.9	5.9	EU RAR (TBBPA)
Koc(l/kg TS)	49726	49726	EU RAR (TBBPA)
KD(l/kg TS)	497	497	0.01 Koc
Henry (-)	-	9.4E-12	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	1200	1234	EU RAR (TBBPA); 1,200 in Fathead minnows (<i>Pimephalus promelas</i>) from EFSA (2011)
BCF stem	-	2.69	
BCF root	-	1055	
MTDI (mg/kg/d)	-	1	EFSA (2011) = 1; REACH chronic = 2.5
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	4.3	REACH = 4.3
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.067	0.0073	REACH Reliability 1 exp
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.67 Bisphenol A

Background parameters and concentrations

Substance	bisphenol A		
CAS #		80-05-7	
M.W. (g/mol)		228	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	3.4	3.4	EU RAR (BPA)
Koc(l/kg TS)	1349	715	EU RAR (BPA)
K_D(l/kg TS)	13	7.15	0.01 Koc
Henry (-)	1.1E-11	1.3E-10	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	5.1	67	EU RAR (BPA) 155 estimated from Pow
BCF stem	-	4.27	
BCF root	-	13.4	
MTDI (mg/kg/d)	0.05	1	M-241 = 1; REACH chronic (acute = 0.004) = 0.004
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	1	REACH = 1
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0.093	REACH Reliability 1 exp
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.68 PFOS

Background parameters and concentrations

Substance	PFOS		
CAS #		1763-23-1	
M.W. (g/mol)		500.13 (som syre)	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	6.4 in Neutral form. -5.0 at pH 8 (Wang et al. 2011)
Koc(l/kg TS)	2690	1000	Zareitalabad et al. (2013)
K_D(l/kg TS)	26.9	10	0.01×Koc, assuming 1% TOC in soil
Henry (-)	0.000000032	8.7x10 ⁻¹⁰ (pH =4)	log Kaw = -1.7 (neutral form). -13.1 at pH 8 (Wang et al., 2011)
BCF fish (l/kg w.w.)	2796	2796	EU dossier PFOS (2011)
BCF stem (l/kg w.w.)	-	0.17	K _D × empirical conc. leaf/conc. soil (Wintersen et al., 2019)
BCF root (l/kg w.w.)	-	0.01	K _D × empirical conc. root/conc. soil (Wintersen et al., 2019)
MTDI (mg/kg/d)	0.0001	1.86 x 10⁻⁶	EFSA (2018)
Proposed MTDI		1.14 x 10⁻⁶	sum PFOS, PFHxS, PFOA, PFNA EFSA (2020)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.69 Nonylphenols and their ethoxylates

Background parameters and concentrations

Substance	nonylphenols (including ethoxylates)		
CAS #	84852-15-3		
M.W. (g/mol)	220		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.48	4.48	EU dossier (NP)
Koc(l/kg TS)	6596	5360	EU dossier (NP)
K_D(l/kg TS)	66	53.6	0.01 Koc
Henry (-)	0.00011	0.004	REACH Reliability 2
BCF fish (l/kg w.w.)	-	1280	EU dossier (NP)
BCF stem	-	6.40	
BCF root	-	85.9	
MTDI (mg/kg/d)	-	0.05	Johnsson (2008) = 0.05
MTDI cancer (mg/kg/d)	-	-	REACH chronic = 0.4 (acute = 0.8) - (Phenol, 4-nonyl-, branched)
RfC (mg/m³)	-	0.4	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0.001	REACH Reliability 2 exp, median used (0,1;0,1;0,12)
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.70 Octylphenols and their ethoxylates

Background parameters and concentrations

Substance	octylphenols (including ethoxylates)		
CAS # M.W. (g/mol)	140-66-9 (1806-26-4) 206		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.12	4.12	variable (3 - 5.7), EU dossier (OP)
Koc(l/kg TS)	2740	2740	variable (2740 - 18400 in dossier)
K_D(l/kg TS)	25	27.4	0.01 Koc
Henry (-)	0.0000085	0.079	REACH Reliability 2 4-(1,1,3,3-tetramethylbutyl)phenol
BCF fish (l/kg w.w.)	6.34	634	variable (471 - 6000), worst case used
BCF stem	-	6.15	
BCF root	-	45.7	
MTDI (mg/kg/d)	-	0.000000067	Jonsson (2008); Eu dossier (OP) verdi er 150. = 0.000000067
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	0.6	REACH chronic AF 50 = 0.6, (acute = 1.8) - 4-(1,1,3,3-tetramethylbutyl)phenol6
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0.0008	REACH Reliability 2 read across, median used (0,07;0,08;0,14)
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.71 Tributyltin compounds

Background parameters and concentrations

Substance	tributyltin compounds		
CAS # M.W. (g/mol)	688-73-3; 366643-28-4 290		
Property	2011 Values	New Review	References for new values and notes
log Pow (l/l)	3.2	4.4	3.1 - 4.4 from EU dossier and Arnold et al. (1997)
Koc(l/kg TS)	2000	1084	conservative log Koc 2.5 - 6.1 dossier, field 5.1 to 5.7 (Berg et al. (2001))
K_D(l/kg TS)	20	10.8	0.01 Koc
Henry (-)	0.0000017	0.0000017	
BCF fish (l/kg w.w.)	2600	6000	EU dossier (TBT)
BCF stem	1.1	6.40	
BCF root	1.1	74.6	
MTDI (mg/kg/d)	0.0003	0.00025	EU dossier (TBT) = 0.00025
MTDI cancer (mg/kg/d)	0.00025	0.00025	
RfC (mg/m³)		-	
RfC cancer (mg/m³)		-	
Skin contact: f_{du}	0	0.151	REACH Reliability 2 exp, median used
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.72 Triphenyltin compounds

Background parameters and concentrations

Substance	Triphenyltin compounds		
CAS # M.W. (g/mol)		892-20-6, 900-95-8, 76-87-9, 639-58-7 350	
Property	2011 Values	New Review	References for new values and notes
log Pow (l/l)	-	3.43	3.43 WHO (1999), 3.1 USEPA (1999)
Koc(l/kg TS)	2000	1900	1900 – 54000 (USEPA, 1999)
K _D (l/kg TS)	20	19	0.01 Koc
Henry (-)	0.00000063	0.00000063	
BCF fish (l/kg w.w.)	1100	1100	257 – 4100 (WHO, 1999), 530 – 7500 with 1100 suggested (Aquateam, 2011)
BCF stem	0	4.37	
BCF root	0	14.0	
MTDI (mg/kg/d)	0	0.00025	EFSA (2004), (VKM, 2007) = 0.00025
MTDI cancer (mg/kg/d)	0.00025	0.00025	
RfC (mg/m ³)		-	
RfC cancer (mg/m ³)		-	
Skin contact: f _{du}	0	0	
Background			
Freshwater (µg/L)	-	0	0
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	m.d	m.d	

4.73 DEHP

Background parameters and concentrations

Substance	DEHP		
CAS #		117-81-7	
M.W. (g/mol)		391	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.1	7.5	EU dossier (DEHP)
Koc(l/kg TS)	-	165000	variable 63100 - 88800 (depends on cation)
K_D(l/kg TS)	5860	1650	0.01 Koc
Henry (-)	0.000044	0.000044	worst case BCF EU RAR (DEHP): 840 (fish), 2500 (mussels), 2700 crustaceans
BCF fish (l/kg w.w.)	840	840	
BCF stem	-	0.14	
BCF root	-	17990	
MTDI (mg/kg/d)	0.02	0.048	RIVM (2001) = 0.048
MTDI cancer (mg/kg/d)	0.004	0.004	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0,00064	REACH Reliability 2 exp, NB! total amount migrated from film to skin and bandaging was 0,064%
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.74 MCCP

Background parameters and concentrations

Substance	MCCP		
CAS #	85535-85-9		
M.W. (g/mol)	232.5-826.5		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.58	7	UK Environment Agency (MCCP)
Koc(l/kg TS)	91201	7616755	Log Koc = 0,00028 + 0,9831logPow
K_D(l/kg TS)	912	76168	0.01 Koc
Henry (-)	-	-	
BCF fish (l/kg w.w.)	1087	1087	variable EU RAR (MCCP)
BCF stem	-	0.44	
BCF root	-	7414	
MTDI (mg/kg/d)	-	0.004	Lowest NOAEL 0.4 mg/kg bw/day EU RAR (MCCP), AF = 100 = 0.004; REACH chronic = 0.58
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	2	REACH = 2
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0.007	REACH Reliability 1 exp
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.75 SCCP

Background parameters and concentrations

Substance	SCCP		
CAS #		85535-84-8	
M.W. (g/mol)		337	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	4.39	6	funciton of Chlorine content (6 used by the EU dossier (SCCP))
Koc(l/kg TS)	199500	199526	EU dossier (SCCP)
K_D(l/kg TS)	1995	1995	0.01 Koc
Henry (-)	-	-	
BCF fish (l/kg w.w.)	-	1600	1173 - 7816 (whole fish), 24000 - 40900 (mussels)
BCF stem	-	2.38	
BCF root	-	1260	
MTDI (mg/kg/d)	-	0.1	UNEP Stockholm Convention (2012) SCCP = 0.1; REACH chronic = 2.5
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	8.7	REACH = 8.7
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0.0001	REACH Reliability 2 exp, less than 0,01%
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.76 Polychlorinated naphthalenes

Background parameters and concentrations

Substance	polychlorinated naphthalenes		
CAS # M.W. (g/mol)		n.a. n.a.	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
KD(l/kg TS)	-	-	
Henry (-)	-	-	
BCF fish (l/kg w.w.)	-	-	
BCF stem	-	-	
BCF root	-	-	
MTDI (mg/kg/d)	-	0.08	RIVM (2001) = 0.08
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	-	-	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	0.000317 (U.K.)	0.000317 (U.K.)	

4.77 Tricresyl phosphate

Background parameters and concentrations

Substance	tricresyl phosphate		
CAS #		1330-78-5	
M.W. (g/mol)		368.37	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	5.11	5.93	REACH Reliability 2
Koc(l/kg TS)	29512	20417	REACH Reliability 1
K_D(l/kg TS)	295	204	0.01 Koc
Henry (-)	0.0000011	0.0000011	
BCF fish (l/kg w.w.)	2768	21903	calculated EU-TGD (2011)
BCF stem	-	2.60	
BCF root	-	1113	
MTDI (mg/kg/d)	-	0.05	REACH chronic = 0.05
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	0.08	REACH = 0.08
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.78 Dioxins

Background parameters and concentrations

Substance	dioxins		
CAS #		1746-01-6	
M.W. (g/mol)		321.97	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	6.8	2,3,7,8-TCDD (EPISuite)
Koc(l/kg TS)	1400000	4500000	eq
K_D(l/kg TS)	14000	45000	0.01 Koc
Henry (-)	0.0003	0.0003	
BCF fish (l/kg w.w.)	-	41540	EU dossier (dioxin)
BCF stem	-	0.66	
BCF root	-	5201	
MTDI (mg/kg/d)	1.4E-09	2E-09	1 to 4 pg TEQ/kg/dag = 0.000000002
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	0.2	0.2	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.79 D5

Background parameters and concentrations

Substance	D5		
CAS #		541-02-6	
M.W. (g/mol)		371	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	8.03	UK Environment Agency (D5)
Koc(l/kg TS)	-	150000	UK Environment Agency (D5)
K_D(l/kg TS)	-	1500	0.01 Koc
Henry (-)	-	1349	REACH Reliability 2
BCF fish (l/kg w.w.)	-	7060	Variabel. UK Environment Agency (D5)
BCF stem	-	0.033	
BCF root	-	46037	
MTDI (mg/kg/d)	-	0.25	UK Environment Agency RAR D5. Oral LOAEL 25 mg/kg kroppsvikt/day og AF 100. = 0.25; REACH chronic =5 (acute = 5)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	17.3	REACH (local 4.3 mg/m ³) = 17.3
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.80 PFOA

Background parameters and concentrations

Substance	PFOA		
CAS # M.W. (g/mol)	3825-26-1. flere 414.07 (as acid)		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	2.2	5.3 in Neutral form, -1.8 at pH 8, 2.2 at pH 4 (Wang et al. 2011)
Koc(l/kg TS)	-	125	Zareitalabad et al. (2013)
K_D(l/kg TS)	-	1.25	0.01×Koc, assuming 1% TOC in soil
Henry (-)	-	1.0×10^{-3}	log Kaw = -3.0 (Li et al. 2007), calculated -1.9 neutral form, -9.0 at pH 8
BCF fish (l/kg w.w.)	-	4.0	1.8 – 8.0 for different fish species (ECHA, 2013)
BCF stem (l/kg w.w.)	-	0.044	K _D × empirical conc. leaf/conc. soil (Wintersen et al., 2019)
BCF root (l/kg w.w.)	-	0.015	K _D × empirical conc. root/conc. soil (Wintersen et al., 2019)
MTDI (mg/kg/d)	-	0.86×10^{-6}	EFSA (2018)
Proposed MTDI		1.14×10^{-6}	sum PFOS, PFHxS, PFOA, PFNA EFSA (2020)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-		
Coastal water (µg/L)	-		
Sediment (mg/kg)	-		
Soil (mg/kg)	-	-	

4.81 Triclosane

Background parameters and concentrations

Substance	triclosane		
CAS #		3380-34-5	
M.W. (g/mol)		290	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	4.76	WFD-UKTAG (2009), Environment Canada (2012), ECHA data base = 4.9
Koc(l/kg TS)	-	900	
K _D (l/kg TS)	-	9	0.01 Koc
Henry (-)	-	4.0E-07	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	-	8700	
BCF stem	-	6.14	
BCF root	-	141	
MTDI (mg/kg/d)	-	0.25	= 0.25
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	-	0.072	REACH Reliability 1 exp
Background			
Freshwater (µg/L)	-	0	0
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	-	-	

4.82 TCEP

Background parameters and concentrations

Substance	TCEP		
CAS # M.W. (g/mol)		115-96-8 (CAS TA-3001 brukes til tris(2-carboxyethyl)phosphine) 285	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	1.78	EU RAR (TCEP)
Koc(l/kg TS)	-	110	EU RAR (TCEP)
K _D (l/kg TS)	-	1.1	0.01 Koc
Henry (-)	-	-	
BCF fish (l/kg w.w.)	-	5.1	Largest value EU RAR (TCEP)
BCF stem	-	1.0	
BCF root	-	1.53	
MTDI (mg/kg/d)	-	0.12	LOAEL (12000) AF (100) – EU RAR (TCEP)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	-	
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	-	-	
Background			
Freshwater (µg/L)	-	0	0
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	-	-	

4.83 Dodecylphenols

Background parameters and concentrations

Substance	dodecylphenols		
CAS # M.W. (g/mol)	121158-58-5, 27193-86-8 262		
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	7.14	UK Environment Agency (dodecylphenol)
Koc(l/kg TS)	-	110000	UK Environment Agency (dodecylphenol)
K _D (l/kg TS)	-	1100	0.01 Koc
Henry (-)	-	-	
BCF fish (l/kg w.w.)	-	823	UK Environment Agency (dodecylphenol)
BCF stem	-	0.33	
BCF root	-	9502	
MTDI (mg/kg/d)	-	0.05	UK Environment Agency (dodecylphenol) NOAEL = 5000, AF = 100 = 0.05; REACH chronic = 0.075 (acute = 1.26)
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	0.79	REACH (acute = 13.26 mg/m ³) = 0.79
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	-	-	
Background			
Freshwater (µg/L)	-	0	0
Coastal water (µg/L)	-	0	
Sediment (mg/kg)	-	0	
Soil (mg/kg)	-	-	

4.84 Diuron

Background parameters and concentrations

Substance	diuron		
CAS #		330-54-1	
M.W. (g/mol)		233	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	2.8	EU dossier (diuron)
Koc(l/kg TS)	-	355	EU dossier (diuron)
K_D(l/kg TS)	-	3.55	0.01 Koc
Henry (-)	-	8.2E-10	REACH Reliability 2 (estimated)
BCF fish (l/kg w.w.)	-	2	EU dossier (diuron)
BCF stem	-	2.51	
BCF root	-	5.15	
MTDI (mg/kg/d)	-	0.007	EU dossier (diuron) = 0.007
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.85 Irgarol

Background parameters and concentrations

Substance	irgarol		
CAS #		28159-98-0	
M.W. (g/mol)		253	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	4	EU dossier (irgarol)
Koc(l/kg TS)	-	1400	EU dossier (irgarol)
K_D(l/kg TS)	-	14	0.01 Koc
Henry (-)	-	-	
BCF fish (l/kg w.w.)	-	250	EU dossier (irgarol)
BCF stem	-	5.94	
BCF root	-	37.1	
MTDI (mg/kg/d)	-	0.023	EU dossier (irgarol) = 0.023
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	-	
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.86 Antimony

Background parameters and concentrations

Substance	antimony		
CAS #		7440-36-0	
M.W. (g/mol)		121.760	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	-	
Koc(l/kg TS)	-	-	
K _D (l/kg TS)	-	38	EU RAR (antimony)
Henry (-)	-	-	
BCF fish (l/kg w.w.)	-	-	-
BCF stem	-	-	
BCF root	-	-	
MTDI (mg/kg/d)	-	140.8	REACH chronic = 140.8
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m ³)	-	0.1	REACH = 0.1
RfC cancer (mg/m ³)	-	-	
Skin contact: f _{du}	-	0.0026	REACH Reliability 1 read across
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.87 Galaxolide

Background parameters and concentrations

Substance	galaxolide		
CAS #		1222-05-5	
M.W. (g/mol)		258.40	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	5.4	REACH Reliability 2
Koc(l/kg TS)	-	8710	REACH Reliability 2 (estimated)
K_D(l/kg TS)	-	87	0.01 Koc
Henry (-)	-	0.015	REACH Reliability 2
BCF fish (l/kg w.w.)	-	7762	calculated EU-TGD (2011)
BCF stem	-	4.40	
BCF root	-	435	
MTDI (mg/kg/d)	-	3.8	REACH chronic = 3.8
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	0.043	REACH (acute = 0.131) = 0.043
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	0.052	REACH Reliability 2 exp
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

4.88 Tonalide

Background parameters and concentrations

Substance	tonalide		
CAS #		21145-77-7	
M.W. (g/mol)		258.405	
Property	2007 Values	New Review	References for new values and notes
log Pow (l/l)	-	5.3	REACH Reliability 2
Koc(l/kg TS)	-	24547	REACH Reliability 2 (estimated)
K_D(l/kg TS)	-	245	0.01 Koc
Henry (-)	-	0.015	REACH Reliability 2
BCF fish (l/kg w.w.)	-	6383	calculated EU-TGD (2011)
BCF stem	-	4.74	
BCF root	-	365	
MTDI (mg/kg/d)	-	3.8	REACH chronic = 3.8
MTDI cancer (mg/kg/d)	-	-	
RfC (mg/m³)	-	6.5	REACH = 6.5
RfC cancer (mg/m³)	-	-	
Skin contact: f_{du}	-	-	
Background			
Freshwater (µg/L)	-	-	
Coastal water (µg/L)	-	-	
Sediment (mg/kg)	-	-	
Soil (mg/kg)	-	-	

5 Summary table of compound specific parameters

Summary of the reviewed background parameters relevant for the estimation of health effects according to the Norwegian guidelines for risk assessment and the worksheet tool, that is using these compound specific parameters, available at <http://www.miljodirektoratet.no/>.

Table 2 Summary of key parameters needed to assess the risk for human health from the review of the literature conducted in this report.

Substance	Henry	Kd (l/kg)	Koc (l/kg)	log Pow	BCF fish	BCF stem	BCF root	MTDI (mg/kg/d)	MTDI cancer risk (mg/kg/d)	RfC (mg/m ³)	RfC cancer risk (mg/m ³)	Skin contact f _{du}
Arsenic	-	6607	-	-	4	0.03	0.015	0.0003	-	0.0025	0.0000067	0.03
Lead	-	154882	-	-	424	0.03	0.001	0.00108	-	0.00015	-	0.0009
Cadmium	-	130000	-	-	623	0.7	0.15	0.00015	-	0.000005	0.0000056	0.14
Mercury	0.3	100000	-	-	200	0.03	0.015	0.00222	-	0.004	-	0.05
Copper	-	24409	-	-	200	0.1	0.1	0.163	-	-	-	0.112
Zink	-	110000	-	-	1000	0.4	0.1	0.5	-	2.5	-	0.02
Chromium (III)	-	11000	-	-	200	0.02	0.002	0.0015	-	0.5	-	0.04
Chromium (VI)	-	30	-	-	200	0.02	0.002	0.0015	-	0.000008	0.00000025	0.09
Chromium total (III + VI)	-	11000	-	-	50	0.002	0.02	0.0015	-	0.027	0.000003	0.09
Nickel	-	7079	-	-	270	0.1	0.07	0.015	-	0.000025	0.000012	0.35
Cyanide	0.005	0.028	2.8	-0.25	0.12	0.12	0.84	0.012	-	0.025	-	0.3
PCB 7	0.00034	3211	321119	5.72	24950	200	200	0.00001	0.0000013	-	-	0.067
lindane	0.00000292	37	3715	3.5	1300	0.15	0.86	0.001	0.0000075	-	0.000026	-
DDT	0.0023	62159	6215857	6.91	30000	0.05	0.002	0.01	0.000029	-	0.007	-
monochlorobenzene	0.15	4	398	2.89	57	2.74	5.89	0.2	-	1	0.071	0.1
1,2-dichlorobenzene	0.079	4	398	3.43	164	4.37	14.0	0.43	-	1	-	0.1
1,4-dichlorobenzene	0.10	3.7	372	3.37	146	4.17	12.7	0.1	0.0004	8.2	-	0.1

Substance	Henry	Kd (l/kg)	Koc (l/kg)	log Pow	BCF fish	BCF stem	BCF root	MTDI (mg/kg/d)	MTDI cancer risk (mg/kg/d)	RfC (mg/m ³)	RfC cancer risk (mg/m ³)	Skin contact f _{du}
trichlorobenzenes	0.0039	14	1400	4.05	1140	6.04	40.5	0.008	-	0.008	-	0.08
1,2,4,5-tetrachlorobenzene	0.54	59	5888	4.6	4830	6.22	126.4	0.0003	-	-	-	0.1
pentachlorobenzene	0.15	400	40000	5.2	5300	5.06	306	0.0005	-	-	-	0.1
hexachlorobenzene	0.0064	1300	130000	5.7	42000	3.36	740	0.00016	0.000033	0.003	0.00075	0.13
dichloromethane	0.11	0.088	8.8	1.3	2.54	0.69	1.12	0.06	0.0013	88.3	0.05	0.1
trichloromethane	0.11	1.9	185	1.97	13	1.15	1.81	0.03	0.000164	0.18	0.024	0.1
trichloroethene	0.42	1.4	141	2.5	28	1.92	3.50	0.05	-	0.023	-	0.1
tetrachloromethane	1.21	0.8	84.1	2.83	51	2.58	5.38	0.004	-	0.107	-	0.00046
tetrachloroethene	0.87	1.4	141	2.53	28	1.92	3.50	0.016	0.0002	34.5	0.0055	0.1
1,2-dichloroethane	0.045	1.2	116	1.45	2	0.77	1.21	0.014	0.00012	0.0029	0.0036	1
1,2-dibromoethane	0.03	0.41	40.7	1.96	9.2	1.14	1.80	-	0.000035	1.15	0.00005	0.1
1,1,1-trichloroethane	0.0007	1.1	110	2.5	27	1.86	3.36	0.58	-	0.8	-	0.1
1,1,2-trichloroethane	0.04	0.8	80	2.27	17	1.49	2.51	0.004	-	-	-	-
phenol	0.000013	0.3	30	1.47	3.5	0.79	1.23	0.04	-	1.32	-	0.8
sum mon-tetrachlorophenols	0.00004	0.3	30	3.7	279	5.20	22.2	0.003	-	-	-	0.26
pentachlorophenol	0.000226	34	3400	3	770	3.04	247	0.003	0.000083	-	0.0000075	0.11
naphthalene	0.0117	13	1349	3.3	515	3.95	11.3	0.04	-	0.003	-	0.83
acenaphthylene	0.029	26	2570	3.55	509	4.74	17.2	0.05	-	-	-	0.18
acenaphthene	0.011	51	5129	3.92	1000	5.77	32.3	0.5	-	-	-	0.2
phenanthrene	0.00135	372	37154	4.502	4751	6.39	89.2	0.04	-	-	-	0.18
anthracene	0.0021	295	29512	4.68	3042	6.25	122	0.04	-	-	-	0.2
fluorene	0.00619	102	10233	4.18	1658	6.24	50.8	0.04	-	-	-	0.2
fluoranthene	0.00163	977	97724	5.2	4800	5.06	306	0.05	-	-	0.000012	0.2
pyrene	0.0000749	589	58884	4.96	88157	5.73	200	0.5	-	-	-	0.2

Substance	Henry	Kd (l/kg)	Koc (l/kg)	log Pow	BCF fish	BCF stem	BCF root	MTDI (mg/kg/d)	MTDI cancer risk (mg/kg/d)	RfC (mg/m ³)	RfC cancer risk (mg/m ³)	Skin contact f _{du}
benzo(a)anthracene	0.0000017	5012	501187	5.91	33457	2.66	1074	0.005	0.00023	-	0.0000077	0.2
chrysene	0.0000047	3981	398107	5.81	6088	2.99	900	0.05	0.0023	-	0.0000012	0.2
benzo(b)fluoranthene	0.0000028	8319	831864	5.78	11138	3.09	853	0.005	0.00023	-	0.00000083	0.2
benzo(k)fluoranthene	0.0000028	7943	794328	6.11	11138	2.06	1531	0.005	0.00023	-	0.0000012	0.2
benzo(a)pyrene	0.000034	8318	831764	6.11	11138	2.06	1531	0.0005	0.00001	-	0.00000011	0.2
indeno(1,2,3-cd)pyrene	0.00000117	23442	2344229	6.7	11138	0.80	4356	0.005	0.00023	-	0.0000005	0.18
dibenzo(a,h)anthracene	0.000038	19498	1949845	6.55	50119	1.05	3339	0.0005	0.000023	-	0.000000023	0.09
benzo(g,h,i)perylene	0.000004	10233	1023293	6.63	11138	0.91	3848	0.03	-	-	-	0.18
PAH totalt	0.0000749	589	58884	4.96	88157	5.73	200	see BaP	see BaP	-	see BaP	0.2
benzene	0.159	1.3	134	2.13	13	1.31	2.14	0.007	0.00033	0.05	0.0012	0.015
toluene	0.27	0.64	63.8	2.73	42	2.34	4.64	0.223	-	56.5	-	0.036
ethylbenzene	0.33	2.5	250	3.6	229	4.90	18.7	0.1	-	15	-	0.2
xylene	0.26	2.5	250	3.2	105	3.64	9.61	0.15	-	14.8	-	0.118
aliphatics C5-C6	47	8	800	3.3	122	3.88	10.9	2	-	18.4	-	1
aliphatics > C6-C8	50	40	4000	4.0	488	5.92	36.3	2	-	18.4	-	1
aliphatics > C8-C10	55	320	32000	4.9	2841	5.90	176	0.1	-	1	-	0.5
sum aliphatics > C5-C10	34	-	-	3.9	412	5.72	31.2	0.1	-	1	-	0.2
aliphatics > C10-C12	60	2500	250000	5.8	16272	3.09	850	0.1	-	1	-	0.5
aliphatics > C12-C35	87	1.0E+07	1.0E+09	6.3	40179	1.57	2144	2	-	1	-	0.1
MTBE	0.022	0.06	6	1.23	2	0.66	1.09	7.1	-	53.6	-	0.002
tetraethyl-lead	0.19	13	1300	4.385	1065	6.39	72.7	1E-07	-	0.08	-	0.065
brominated diphenylethers	1.2E-06	5659	565860	6.5	35000	1.14	3056	1.4E-07	-	-	-	0.067
PBDE-209	4.9E-07	5.25E+09	5.25E+11	9.9	637	3.3E-05	1.27E+06	20	-	70	-	0.067
HBCDD	0.000117	457	45709	5.62	18100	3.64	643	0.1	-	0.719	-	0.0001

Substance	Henry	Kd (l/kg)	Koc (l/kg)	log Pow	BCF fish	BCF stem	BCF root	MTDI (mg/kg/d)	MTDI cancer risk (mg/kg/d)	RfC (mg/m ³)	RfC cancer risk (mg/m ³)	Skin contact f _{du}
tetrabromobisphenol A	9.4E-12	497	49726	5.9	1234	2.69	1055	1	-	4.3	-	0.0073
bisphenol A	1.3E-10	7.15	715	3.4	67	4.27	13.4	1	-	1	-	0.093
PFOS	8.7E-10	10	1000	-	2796	0.17	0.01	1.86E-06	-	-	-	-
nonylphenols	0.004	53.6	5360	4.48	1280	6.40	85.9	0.05	-	0.4	-	0.001
octylphenols	0.079	27.4	2740	4.12	634	6.15	45.7	6.7E-08	-	0.6	-	0.0008
tributyltin compounds	1.7E-06	10.8	1084	4.4	6000	6.40	74.6	0.00025	0.00025	-	-	0.151
triphenyltin compounds	6.3E-07	19	1900	3.43	1100	4.37	14	0.00025	0.00025	-	-	-
DEHP	4.4E-05	1650	165000	7.5	840	0.14	17990	0.048	0.004	-	-	0.00064
MCCP	-	76168	7616755	7	1087	0.44	7414	0.004	-	2	-	0.007
SCCP	-	1995	199526	6	1600	2.38	1260	0.1	-	8.7	-	0.0001
polychlorinated naphthalenes	-	-	-	-	-	-	-	0.08	-	-	-	-
tricresyl phosphate	1.1E-06	204	20417	5.93	21903	2.60	1113	0.05	-	0.08	-	-
dioxins	0.0003	45000	4500000	6.8	41540	0.66	5201	2E-09	-	-	-	0.2
D5	1349	1500	150000	8.03	7060	0.033	46037	0.25	-	17.3	-	-
PFOA	0.001	1.25	125	2.2	4.0	0.044	0.015	0.86E-06	-	-	-	-
triclosane	4.0E-07	9	900	4.76	8700	6.14	141	0.25	-	-	-	0.072
TCEP	-	1.1	110	1.78	5.1	1.0	1.53	0.12	-	-	-	-
dodecylphenols	-	1100	110000	7.14	823	0.33	9502	0.05	-	0.79	-	-
diuron	8.2E-10	3.55	355	2.8	2	2.51	5.15	0.007	-	-	-	-
irgarol	-	14	1400	4	250	5.94	37.1	0.023	-	-	-	-
antimony	-	38	-	-	-	-	-	140.8	-	0.1	-	0.0026
galaxolide	0.015	87	8710	5.4	7762	4.40	435	3.8	-	0.043	-	0.052
tonalide	0.015	245	24547	5.3	6383	4.74	365	3.8	-	6.5	-	-

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