CHEMICAL SAFETY REPORT

Legal name of applicant(s):	Rain Carbon bvba
Submitted by:	Rain Carbon bvba
Substance:	1. Pitch, coal tar, high-temp., EC 266-028-2, CAS 65996-93-2 2. Anthracene oil, EC 292-602-7, CAS 90640-80-5
Use title:	1A. Use of CTPht for manufacture of formulations for various industrial uses *1B:* Use of AO for manufacture of formulations for various industrial uses
Use number:	*1A, 1B*

Content

Part B

9 EXPOSURE ASSESSMENT (AND RELATED RISK CHARACTERISATION)

9.0 Introduction

9.0.1 Remarks on scope of assessment

With Commission Regulation (EU) 2017/999 of 13 June 2017 pitch, coal tar, high temp. (EC No: 266-028-2 CAS No: 65996-93-2) as well as anthracene oil (EC No: 292-602-7 CAS No: 90640-80-5) have been included into Annex XIV of Regulation (EC) No 1907/2006.

Both substances have been included due to their carcinogenic (Cat 1B) and PBT/vPvB properties. The entry for anthracene oil in the Commission Regulation contains the following footnote:

"Does not meet the criteria for identification as a carcinogen if it contains <0.005% (w/w) benzo[a]pyrene (EINECS No 200-028-5)".

According to Article 62 (4)(d) of REACH, the CSR supporting an Application for Authorisation (AfA) needs to cover only those risks arising from the intrinsic properties specified in Annex XIV. As the anthracene oil with the CAS No. 90640-80-5 produced and used as described in this CSR does contain benzo[a]pyrene in concentrations below 0.005% only, anthracene oil (EC No: 292-602-7 CAS No: 90640-80-5) is not considered a carcinogen in this CSR and, in consequence, human health risks of workers and of humans via the environment are not addressed for this substance in this CSR.

To summarise, the following endpoints are considered:

- Coal tar pitch, high temp. (CTPht, EC No: 266-028-2 CAS No: 65996-93-2)
  - Carcinogenicity (for workers as well as human exposure via the environment)
  - Environmental assessment due to PBT/vPvB properties
- Anthracene oil (AO, EC No: 292-602-7 CAS No: 90640-80-5)
  - Environmental assessment due to PBT/vPvB properties

9.0.2 Overview of uses and Exposure Scenarios

This CSR is part of the application for authorisation for the uses listed in the following table.

A detailed process description including information on tonnages used is provided in section 9.1.

Table 9-1: Overview of CTPht uses applied for and their exposure scenarios

Identifiers *	Titles of exposure scenarios
F-1	Use of CTPht for manufacture of formulations for various industrial uses
* Formulation: F-#	

For the contributing scenarios contained in this ES, see sections 9.1.

Table 9-2: Overview of AO uses applied for and their exposure scenarios

Identifiers *	Titles of exposure scenarios
F-1	Use of AO for manufacture of formulations for various industrial uses
* Formulation: F-#	

For the contributing scenarios contained in this ES, see section 9.1.

Note that CTPht and AO are used at the same site and environmental emissions of PAHs from use of these substances cannot be separated. Therefore, one environmental contribution scenario covering emissions from both substances was prepared for the formulation use.

9.0.3 Introduction to the assessment

9.0.3.1 Environment

Scope and type of assessment:

As explained above and in more detail in chapter 8, in addition to its carcinogenic activity, CTPht is listed in Annex XIV of REACH due to the presence of PAH-constituents classified vPvB and/or PBT in concentrations over 0.1%. According to the SVHC Support Document (ECHA, 2009c), seven PAH-constituents present in CTPht fulfil both, the vPvB and the PBT criterion. In addition, phenanthrene fulfils the vPvB, and anthracene the PBT criterion (ECHA, 2009a; b).

AO is considered as a substance with vPvB and PBT properties, due to the presence of constituents classified vPvB and/or PBT: anthracene, fluoranthene, pyrene and phenanthrene (ECHA, 2009a; b).

The nine PAHs considered as PBT and/or vPvB substances in the SVHC Support Document for CTPht (ECHA, 2009c) are given in the following table (for a critical discussion of data underlying the PBT/vPvB evaluation, especially with regard to bioaccumulation, see section 4).

Table 9-3: Overview on PBT/vPvB conclusions for nine PAHs contained in CTPht or AO according to the SVHC Support Document (ECHA, 2009c)

Substance	Persistence	Bioaccu-mulation	Toxicity Human health	Toxicity Aquatic Environment	Conclusion	in CTPht	in AO
Anthracene	vP	B	-	T	PBT	X	X
Phenanthrene *	vP	vB	-	-	vPvB	X	X

Fluoranthene *	vP	vB	-	T	PBT/vPvB	X	X
Pyrene *	vP	vB	-	T	PBT/vPvB	X	X
Benz[a]anthracene	vP	vB	T	T	PBT/vPvB	X	
Chrysene	vP	vB	T	-	PBT/vPvB	X	
Benzo[a]pyrene	vP	vB	T	T	PBT/vPvB	X	
Benzo[k]fluoran-thene *	vP	vB	T	T	PBT/vPvB	X	
Benzo[ghi]perylene	vP	vB	-	T	PBT/vPvB	X	
* PBT classification agreed upon in the SVHC-listing process, December 2018							

The environmental assessment focuses on the PAHs considered to be PBT/vPvB substances (Table 9-3) according to the SVHC Support Document (ECHA, 2009c).

According to ECHA (2018) in an AfA CSR for a PBT/vPvB substance it should be demonstrated that measures have been taken to reduce emissions and exposure as much as possible. To this end, this CSR describes that

- all available measures have been implemented to reduce emissions to the environmental media and that
- concentrations in the environmental media caused by these emissions are low.

This will be demonstrated in the following chapters. Site-specific technical and organisational measures in place to reduce emissions are explained in detail. Where emissions to environmental media occur, this will be described in a quantitative manner, using site-specific release data where possible and EUSES (version 2.1) modelling for predicting concentrations of the individual PAHs in environmental media.

In addition to these nine PAHs with PBT and/or vPvB properties, also the environmental distribution of benzo[b]fluoranthene will be modelled, since the oral exposure of man via the environment needs to be assessed (as will be described in the next section 9.0.3.2).

For EUSES modelling, the following general parameters will be used for the individual PAHs:

- The physico-chemical properties of the twelve indicator PAHs are given in Table 9-4,
- The data given in Table 9-5 on the environmental fate properties (chapter 4) and the parameters from the environmental hazard assessment (chapter 7) for the ten PAHs which will be modelled,
- A biomagnification factor of 1 in fish and in predators was selected since biomagnification is not expected (see section 7.5),
- All PAHs were characterized as “not biodegradable” according to the descriptions in section 4.1.2.1 (Table 4-3 and Table 4-4),
- “High production volume” was selected for all PAHs,

- The PNECs shown in Table 7-4. In cases where sufficient toxicity data for benthic/ soil species were absent and PNECs were calculated by equilibrium partitioning in the Annex XV Transitional Dossier (The Netherlands, 2008), equilibrium partitioning was also used in EUSES modelling, deriving the same PNECs as in Table 7-4,
- The detailed, site-specific datasets as explained in the respective contributing scenarios.

Potential burdens to the environment will be discussed and compared to the existing background.

Table 9-4: Physico-chemical properties of the twelve indicator PAHs (ECHA, 2009c; The Netherlands, 2008)

Substance	CAS No.	Molecular formula	Molecular weight [g/mol]	Melting point [°C]	Boiling point [°C]	Water solubility [µg/L]	Log Kow [-]	Vapour pressure [Pa at 25 °C]	Density [kg/L]	Henry's Law constant [Pa m^3/mol at 25 °C]
Anthracene	120-12-7	C14H10	178.2	216.4	342 [e]	47 [a]	4.68 [d]	9.4×10^{-4} [i]	1.283	4.3 [l]
Phenanthrene	85-01-8	C14H10	178.2	100.5	340	974 [a]	4.57 [d]	2.6×10^{-2} [i]	0.980	3.7 [l]
Fluoranthene	206-44-0	C16H10	202.3	108.8	375	200 [a]	5.20 [d]	1.2×10^{-3} [h]	1.252	1.1 [o]
Pyrene	129-00-0	C16H10	202.3	156	360	125 [a]	4.98 [e]	1.0×10^{-3} [i]	1.271	1.4 [n]
Benz[a]anthracene	56-55-3	C18H12	228.3	160.7	435	10.2 [a]	5.91 [d]	7.6×10^{-6} [i]	1.226	0.81 [p]
Chrysene	218-01-9	C18H12	228.3	253.8	448	1.65 [a]	5.81 [d]	5.7×10^{-7} [j]	1.274	0.079 [q]
Benzo[a]pyrene	50-32-8	C20H12	252.3	175	496	1.54 [a]	6.13 [d]	7.3×10^{-7} [j]	1.35	0.034 [o (20 °C)]
Benzo[b]fluoran-thene	205-99-2	C20H12	252.3	168.3	481	1.28 [a]	6.12 [f]	3.3×10^{-6} [k]	-	0.051 [o (20 °C)]
Benzo[k]fluoran-thene	207-08-9	C20H12	252.3	217	480	0.93 [a]	6.11 [d]	1.3×10^{-7} [k]	-	0.043 [o (20 °C)]
Benzo[ghi]pery-lene	191-24-2	C22H12	276.3	277	545 [i]	0.14 [a]	6.22 [d]	1.4×10^{-8} [j]	1.329	0.027 [o (20 °C)]
Dibenzo[a,h]an-thracene	53-70-3	C22H14	278.4	266.6	524	0.82 [b]	6.50 [e]	3.7×10^{-10} [j]	1.282	$1.3.10^{-4}$ [q]

Indeno[1,2,3-cd]pyrene	193-39-5	C22H12	276.3	163.6	536	0.1 [c]	6.58 [f]	1.7 x 10^{-8} [k]	-	0.046 [q]
The data presented above were taken from Mackay et al. (1992). The selected values for water solubility were preferably based on generated column methods (a) and if absent, on shake-flask methods (b) using geometric means ((c) for indeno[1,2,3-cd]pyrene, no data were available, a default value of 0.1 µg/L was used). The selected values for log K_{OW} were preferably based on slow-stirring/generator column (c) or slow-stirring methods (d) using average values. If absent the log K_{OW} values were based on the shake-flask method (e), or - in the absence of data - calculated using ClogP model (f). The selected values for vapour pressure were based on manometry/gas saturation (g), gas saturation (h), gas saturation/effusion (i), effusion method (j) using geometric means or estimated using EPIWIN (k). The selected values for the Henry's Law constant were based on batch/gas stripping/wetted-wall column (l), batch/gas stripping (n), gas stripping (o), batch column (p) using geometric means or when no data were available, constants were calculated using EUSES 2.0 (q).										

Table 9-5: Overview of the environmental fate properties (chapter 4) and parameters from the environmental hazard assessment (chapter 7) used for EUSES modelling

		Bioconcentration factors			Degradation and transformation			
PAH	KOC	BCF in earth-worm [kgwwt/L]	BCF in fish or other aquatic organisms [a]	Key study species	Rate constant for biodegradation in surface water [1/d at 12 °C] [d]	Total rate constant for degradation in bulk sediment [1/d at 12 °C] [d]	Phototransformation - reaction rate constants for reaction with atmospheric OH radicals molecule [cm^3/ molecule/s]	Rate constant for biodegradation in bulk soil [1/d at 12 °C] [d]
Anthracene	2.95E+04	580	4.97E+03	Fish	4.44E-05	1.44E-06	1.30E-10	4.42E-06
Phenanthrene	2.29E+04	450	4.75E+03	Fish	4.44E-05	1.44E-06	3.10E-11	4.42E-06
Fluoranthene	9.77E+04	1 900	2.77E+03	Fish	4.44E-05	9.63E-07 [e]	5.00E-11	1.44E-06
Pyrene	5.89E+04	1 200	1.47E+03	Fish	1.44E-05	9.63E-07 [e]	5.00E-11	1.44E-06

Benz[a]anthracene	5.01E+05	9 800	2.60E+02	Fish	1.44E-05	9.63E-07 [e]	1.22E-10	1.44E-06
Chrysene	3.98E+05	7 800	6.09E+03 [b]	Crustaceans	1.44E-05	9.63E-07 [e]	8.00E-11	1.44E-06
Benzo[a]pyrene	8.32E+05	16 000	6.08E+02	Fish	1.44E-05	9.63E-07 [e]	5.00E-11	1.44E-06
Benzo[b]fluoran-thene	8.32E+05	16 000	3.61E+04 [c]	No experimental data available	1.44E-05	9.63E-07 [e]	1.86E-11	1.44E-06
Benzo[k]fluoran-thene	7.94E+05	15 000	1.32E+04 [b]	Crustaceans	1.44E-05	9.63E-07 [e]	5.36E-11	1.44E-06
Benzo[ghi]perylene	1.02E+06	20 000	2.83E+04 [b]	Crustaceans	1.44E-05	9.63E-07 [e]	8.69E-11	1.44E-06
Source	Table 4-5	Table 4-8	Table 4-7	Table 4-7	calculated from Table 4-3	calculated from Table 4-3	Table 4-1	calculated from Table 4-3

[a] The BCF values from key studies selected by Bleeker and Verbruggen (2009) were used. BCFs from key studies in fish were preferred.

[b] If valid fish data are not available, BCFs from key studies in crustaceans were selected since they seemed to be more reliable than the BCFs calculated by the QSAR applied in EUSES. Although it is stated in the Guidance on Information Requirements and Chemical Safety Assessment Chapter R.7c: Endpoint specific guidance Version 3.0 (ECHA, 2017a) that BCFs determined in crustaceans (i.e. invertebrates other than molluscs) should not be used due to high uncertainties in these data, the experimental data determined in crustaceans were preferred over modelling.

[c] In absence of valid studies in fish or crustaceans, the BCF was modelled in EUSES via QSAR.

[d] The arithmetic mean of the range given in the source table was calculated and used for calculating the rate constant.

[e] The half-live of 1 250 days (given information: >1 250 days) was used for calculating the rate constant.

9.0.3.2 Man via environment (assessment performed for CTPht only)

Scope and type of assessment:

Table 9-6: Type of risk characterisation required for man via the environment, based on exposure to benzo[a]pyrene (BaP) as indicator substance for PAHs (according to ECHA, 2018)

Route of exposure and type of effects	Risk estimate (excess lifetime cancer risk)	Remarks
Inhalation: Systemic Long Term	Lung tumours: 3.0×10^{-5} per ng BaP/m^3 Bladder tumours: 2.1×10^{-5} per ng BaP/m^3	uncertainty due to differences in composition in workplace air compared to environmental exposures
Oral: Systemic Long Term	2.06×10^{-3} per µg PAH4/kg bw/day or 1.43×10^{-3} per µg PAH8/kg bw/day	PAH4 and PAH8: sum of 4 and 8 selected PAHs, resp., according to (EFSA, 2008)

Comments on assessment approach:

Inhalation exposure:

Total cancer risks for inhalation exposure are calculated by adding up risks obtained for the two main tumour locations (lung, bladder). Based on epidemiological evidence, risks for tumours at any other location are considered low compared to these two main sites.

Oral exposure - PAH4 / PAH8:

EFSA in its evaluation of human health risks from occurrence of PAHs in food proposed to use either the sum of 4 selected PAHs or the sum of 8 PAHs as a surrogate for the total sum of PAHs (EFSA, 2008):

4 PAH according to EFSA: Benzo[a]pyrene, chrysene, benz[a]anthracene, benzo[b]fluoranthene

8 PAH according to EFSA: in addition to the 4 above: benzo[k]fluoranthene, benzo[ghi]perylene, dibenz[a,h]anthracene, indeno[1,2,3-cd]pyrene

For assessing oral exposure of humans via the environment an exposure assessment for the 4 PAHs is performed.

Where emissions to the environment occur, potential exposures are described in a quantitative manner, using site-specific release data, where possible, and EUSES (version 2.1) modelling for predicting exposures of humans via the environment on a local and regional scale. Resulting risks are calculated using the dose-response relationship as recommended by RAC for the 4 EFSA PAHs (ECHA, 2018) (see above).

The detailed datasets used for the assessment are explained in the respective contributing scenarios (section 9.1).

9.0.3.3 Workers (assessment performed for CTPht only)

Scope and type of assessment:

Table 9-7: Risk characterisation for workers (according to ECHA, 2018)

Route	Type of effect	Risk estimate	Remarks
Inhalation	Carcinogenicity	Lung tumours: 5.6×10^{-6} per ng BaP/m^3 (40 years of occupational exposure) Bladder tumours: 4×10^{-6} per ng BaP/m^3 (40 years of occupational exposure)	based on workplace air concentrations of BaP as indicator substance for total PAH exposure
	Carcinogenicity	see table below	based on urine biomonitoring concentrations of 1-OH-pyrene as biomarker substance for PAH exposure; biomonitoring does include systemic exposure to PAHs
Dermal	Carcinogenicity	1.3×10^{-3} per ng BaP/cm^2/day	based on local BaP concentration on skin

Note that the exposure-risk relationship in the table above for dermal exposure leads to unrealistic high cancer incidence rates among workers even with infrequent and non-intensive dermal contact with CTPht (see below). See also a recent amendment to RAC's publication on exposure-risk relationships for CTPht (ECHA, 2018).

Table 9-8: Risk characterisation for workers, using 1-hydroxypyrene as biomarker for PAH exposure (according to ECHA, 2018)

Urinary 1-OHP value [µmol/mol creatinine]	Corresp. urinary 1-OHP value [µg/g creatinine]	Converted BaP [µg/m^3]	Cumulative exposure (40 years) [µg * years/m^3]	Excess lung cancer risk in EU workers
100	1 930	8.907	356.288	5.0×10^{-2}
10	19.3	0.799	31.964	4.5×10^{-3}
5	9.65	0.349	13.946	2.0×10^{-3}
2	3.86	0.078	3.135	4.4×10^{-4}

1.13	2.18	0.000	0.000	0.0

The conversion of urinary 1-OHP concentrations into BaP air concentrations is applicable in case the contribution from dermal exposure is considered negligible.

Comments on assessment approach related to toxicological hazard:

Inhalation exposure:

Total cancer risks for inhalation exposure are calculated by adding up risks obtained for the two main tumour locations (lung, bladder). Based on epidemiological evidence, risks for tumours at any other location are considered low compared to these two main sites.

ART modelling (Advanced REACH Tool, v 1.5, https://www.advancedreachtool.com/) was used to estimate exposure concentrations for benzo[a]pyrene for Use # 2.

One input parameter required for ART modelling is the vapour pressure of the substance at the specific process temperature. Murray et al. (1974) examined the temperature-dependency of the vapour pressure of benzo[a]pyrene and other PAHs and established a log-linear relationship, which can be used to calculate VP at various temperatures. Goldfarb and Suuberg (2008) measured the vapour pressure of benzo[a]pyrene in a T range from 120 to 150 °C, confirming the validity of the equation of Murray et al. (1974). The following table compares the measured values with those predicted by Murray's equation

$\log_{10}$ VP = - A/T + B, with A = 6 181 °K and B = 9 601 (unitless).

(The result is obtained in atm and needs to be transformed into Pa.)

Table 9-9: Measured and calculated vapour pressures at various temperatures for benzo[a]pyrene

T [°C]	T [°K]	VP, measured by Knudsen Effusion method (Goldfarb and Suuberg, 2008) [Pa]	VP, calculated according to Murray et al. (1974) [Pa]
119.15	392.3	0.0731	0.0709
120.35	393.5	0.0796	0.0792
124.65	397.8	0.129	0.1172
127.65	400.8	0.167	0.1531
129.15	402.3	0.18	0.1748
132.05	405.2	0.217	0.2252
133.45	406.6	0.273	0.2541
138.35	411.5	0.394	0.3856
138.65	411.8	0.418	0.3954
141.95	415.1	0.494	0.5204
142.35	415.5	0.537	0.5379

145.85	419	0.697	0.7161
146.55	419.7	0.733	0.7578
148.05	421.2	0.785	0.8551
150.65	423.8	0.98	1.0520
150.75	423.9	1.02	1.0604

The table shows that even at 150 °C VP of benzo[a]pyrene does not exceed 1 Pa.

The equation above was used to calculate the vapour pressure for activity-specific process temperatures in the respective contributing workers scenarios. At these low vapour pressures ART assumes that potential aerosol exposure is more relevant and needs to be taken into account in the exposure estimate.

Where biomonitoring data are used, risks for bladder tumours are considered by transforming 1-OH pyrene concentrations into benzo[a]pyrene air concentrations, using the relationship provided by RAC (ECHA, 2018).

Dermal exposure assessment

CTPht is a substance with a melting point in the range of 65 to 150 °C, which solidifies at ambient temperatures. In order to be able to handle it in an industrial environment, it is continuously held at elevated temperatures (typically 220-230 °C). Lower temperatures would give rise to solidification in pipes, vessels and pumps and would cause serious process risks. Therefore, during manufacture and formulation the substance is handled in closed systems. For working in these plant areas and for handling the hot substance (e.g. during sampling) workers are required to wear protection against hot materials. Any contact with the substance would immediately cause burns. Furthermore, any contamination of work clothes and gloves with the deep black substance and mixtures is immediately detected. Therefore, regular contamination of the skin can safely be excluded for most activities and no quantitative dermal exposure estimation is provided in this report for these activities.

In some occasions dermal contact with solidified CTPht is possible (e.g. with solid samples for quality control). Due to the enclosure of PAHs in the solid matrix no significant exposure is expected from these materials. Handling of contaminated objects again is a rare event, but will be discussed in the CSR. A qualitative, and where suitable also a quantitative, assessment of dermal exposure is included in every worker contributing scenario.

9.1 Exposure scenario for use 1: Use of CTPht and AO for manufacture of formulations for various industrial uses

9.1.1 Explanations on use

Market sector: -
Sector of use: SU8
Article categories: n.a.
Environment contributing scenario(s): ERC2
Worker/Consumer contributing scenario(s): PROC3, PROC8b; PROC15; PROC28
Subsequent service life exposure scenario(s): n.a.
Exposure scenario(s) of the uses leading to the inclusion of the substance into the article(s): n.a.

9.1.1.1 Description of use and function of the substance for that use

One of the main activities of Rain Carbon at its production site in Zelzate, Belgium is the refinery of coal tar, leading, among other products, to the manufacture of coal tar pitch – high temperature (CTPht; CAS 65996-93-2) and anthracene oil (AO; CAS 90640-80-5). Rain Carbon produces approximately up to [redacted] (50 000-200 000) t CTPht and up to [redacted] (20 000-100 000) t AO per year. In addition to their own production volume, between approximately [redacted] (50 000-200 000) t of CTPht per year are delivered to Rain Carbon from other EEA countries or are imported from non-EEA countries.

For AO, the possibility of exchange between the different sites of the Rain group is present, but this is much less frequent and quantities are much lower (e.g. for 2017 approximately [redacted] (<1 000) t were delivered to Rain Carbon). Three different grades of AO are produced at the site, all of them falling under the definition of AO, which differ slightly in their anthracene concentration.

Currently, the larger part of the volume of CTPht handled at the site ([redacted] (0-300 000) t per year) is used downstream as an intermediate (e.g. for the production of electrodes for the aluminium industry). These uses are exempted from authorisation and not further considered in this application for authorisation.

[redacted]

A smaller part of CTPht (currently [redacted] (0-20 000) t per year, future maximum expected up to [redacted] (0-20 000) t per year) can be blended with coal tar distillates for the production of special carbon black feedstock (CBF) grades or Söderberg pitches. Use of CBF for production of carbon black and use of Söderberg electrode mass are intermediate uses and so exempted from authorisation.

From the total annual volume of up to [redacted] (20 000-100 000) t AO processed per year at the site, a certain part is used to manufacture EU creosote (EN 13991) on-site; the remaining quantities are sold in mixtures for intermediate uses, which are exempted from the application for authorisation, and in mixtures for export. These remaining quantities are used as follows:

- Up to ± [redacted] (5 000-50 000) t per year for formulation of CBF (transported intermediate)
- Up to ± [redacted] (5 000-50 000) t per year for formulation of mixtures for export out of the EU.

Note that the relevant tonnages of AO given in Table 9-11 are from previous years plus a forecast on 2018, as available at the time of the assessment. Definite data now available for 2018 indicate a slightly lower tonnage of AO used for formulation activities: [redacted] (10 000-50 000) t per year in total ([redacted] (5 000-50 000) t per year for formulation of CBF (transported intermediate) and [redacted] (5 000-50 000) t per year for formulation of mixtures for export out of the EU).

The following tables provide an overview on the tonnages of CTPht and AO, which are subject to this application for authorisation. Certain amounts of the mixtures are sold outside the EEA.

Table 9-10: Tonnages of CTPht per type of mixtures and use area (anticipated future situation, which forms the basis for this AfA)

Mixture type	Tonnage CTPht [t/y]	Export out of EEA [t/y]	Used in EEA (intermediate uses) [t/y]
Pitch mixtures containing CTPht (e.g. for aluminium or carbon/graphite industry)	[redacted] (0-300 000)	[redacted] (40-80%)	[redacted] (60-20%)
CBF (mixture with AO and other substances) + Söderberg Paste (mixtures with other substances)	[redacted] (0-20 000)	[redacted] (up to 5 000)	[redacted] (up to 20 000)

Table 9-11: Tonnages of AO per type of mixtures and use area

Mixture type	Tonnage AO [t/y]	Export out of EEA [t/y]	Used in EEA (intermediate uses) [t/y]
CBF	[redacted] (5 000-50 000)	[redacted] (up to 5 000)	[redacted] (up to 50 000)
Mixtures for export	[redacted] (5 000 to 50 000)	[redacted] (5 000 to 50 000)	[redacted]

9.1.1.2 Process description

Coal tar is purchased from several suppliers within and outside of Europe and delivered to Zelzate (75-85% via ships), where it is distilled on-site. CTPht and AO are produced during the distillation process and stocked in several large storage tanks in the center of the plant, close to the tar refinery. CTPht is stored at 200-230 °C and AO at 50-110 °C.

The volumes of the heated tanks are constantly circulated via pumps over an external heat exchanger in order to ensure a homogenous temperature within the whole tank. Pitch tanks have additional small internal immersion heaters.

During formulation procedures, certain amounts of CTPht ([redacted] (0-300 000) t per year) and/or AO ([redacted](10 000-50 000) t per year) are mixed with other streams of the coal tar distillation (e.g. liquid pitch or oils) in order to obtain the desired composition (according to specified, pre-calculated proportions) of the mixture. The actual mixing operation is done by continuous circulation over the storage tank. The mixture may be stored in this tank for a certain amount of time before it is delivered to customers and replaced by another material.

Dedicated tanks are used for the different AO mixtures: CBF, mixtures for export, EU creosotes.

The production at Rain Carbon runs 24 hours per day; seven days per week and formulation activities are an integral part of the production of the sales products. This means that formulation activities for CTPht and AO run 24/7/365.

No regular maintenance activities occur for the tanks used for the formulation process, only single tanks are shut down when necessary (e.g. for tank replacement; tanks have a lifetime of >30 years). All tanks are subject to a preventive inspection program. In a few cases the properties of the mixture in the tank require an internal inspection every 20 years (VLAREM environmental legislation). Equivalent external testing methods are used to the maximal possible extend. No cleaning of the mixture tanks is taking place.

Rain Carbon is located adjacent to the canal “Zeekanaal Gent-Terneuzen” (to the western side of the plant) in Zelzate (Belgium). The wastewater occurring at Rain Carbon is limited to rain water from the concrete surface under the process equipment and tank farms. Itis not subject to this application for authorisation, since the whole formulation process is waterless (for more details see section 9.1.1.5).

9.1.1.3 Definition of groups of exposed humans

Approximately 187 people are working at Rain Carbon, 30% thereof is supporting, administrative or commercial personnel, which does not enter the production unit itself. Of the remaining employees, only a part contributes to work processes related to formulation activities (see below). Since only formulations containing CTPht are needed to be considered for human exposure, exclusively operations and exposed groups of workers related to CTPht mixtures are included in the assessment.

Description of groups of exposed workers:

Operators

The group of operators involved in the formulation processes consists of 22 (18 + 3 + 1) people working at the tar plant. The 18 people work in six shifts, with three different 8h-shifts per day (morning, afternoon and night shift). Three operators are assigned to each shift whereof one person per team, the chief operator, is in charge of the operation and spends most of his labour time in the control room. He has one operator assisting him to control the plant, the plant operator (involves partly transfer/formulation of AO). The third person is the logistics operator who is responsible for material transfer between the tanks (pumping pitch from one tank to the other/formulation) and the un-/loading operations for ships and trucks. For each position (operator, chief operator and logistics operator), one additional person (one operator, one chief operator and one logistics operator) serves as a substitute/spare worker and occupies a seventh shift (normally day shift but he might also fill gaps in the shift schedule, e.g. when another operator needs to be replaced). One operator, the 22nd person, is dedicated to a small batch unit for oil mixtures (incl. AO, not CTPht).

Laboratory workers:

Eleven people work in the laboratory, one manager (day service, 40 h per week, Mon-Fri), five people in day service (40 h per week, Mon-Fri) and five people in shift (8 h shifts, continuous night shift; one person per shift). The laboratory manager is not involved in the laboratory work with mixtures and therefore not considered to be exposed. The time of the laboratory technicians spent on samples from pitch mixtures containing CTPht only constitutes approximately <50% of their overall working time for the shift, <5% for day service technicians. All technicians are capable to work with all types of samples but some persons are more involved in specific analytical tasks (GC, GC-MS) than others.

Maintenance workers:

In total 30 maintenance workers are employed at Rain Carbon, 21 of them have potential exposure to CTPht. Of these 21 workers, 16 are on day service (8 h per day, 40 h per week) and five persons work 24/7 in a three-shift system. During nights and on weekends, they often receive small tasks to be fulfilled but they can flexibly switch to urgent maintenance duties (e.g. on the production plant) in case they arise.

The maintenance workers have their own mechanical workshop, where they take care of all maintenance works. They have the permitting system for several activities wherein all Environmental Health and Safety (EHS) aspects are covered. However, the time of the maintenance workers spent on tasks related to pitch mixtures is negligible since the technical instruments and measures applied in these processes function very reliably with a rare necessity for maintenance work. There are no regular maintenance shutdowns for the formulation process, tanks only need to be opened or replaced after their lifetime.

The only regular maintenance which may occur is on pumps, valves or loading arms; activities with very low exposure potential. For instance, since all pumps are installed in double or triple, if one pump fails, the backup pump takes over and there is low time

pressure to repair the broken pump and, thus, not a high risk for contamination during the maintenance procedure.

There are detailed records on maintenance activities carried out during the recent years. These records provide evidence that close to no maintenance tasks exist for formulation activities. For instance, only six to seven pumps need to be replaced per year.

Written procedures are available in case that maintenance would be necessary on the technical equipment applied in formulation processes. The procedures contain detailed instructions on e.g. how to proceed in case that a pump needs to be repaired (close the lines, empty and clean the pump, transport the pump to the repair shop,…) or cleaned and what PPE has to be used.

Description of groups of humans exposed via the environment:

Of the staff members of Rain Carbon, 32 persons work regularly on the plant section for formulation of CTPht. Rain Carbon is located adjacent to the canal "Zeekanaal Gent-Terneuzen" (to the western side of the plant; see site map provided in Annex I) in Zelzate (Belgium). Industry is bordering to the canal upstream and downstream of Rain Carbon (chemical industry, steel mill in approximately 3 km distance to the south, multiple chemical plants to the north). On the northern side, in flow direction of the canal, Rain Carbon is located in approximately 100 m distance to the Dutch border. The canal ends in the estuary of the Westerschelde, approximately 20 km distant from the sea.

The plant is surrounded by residential areas of Zelzate to its eastern, western and southern parts while the north-west, north and north-east are areas occupied by small and medium-sized enterprises (SMEs) and adjacent to these, rather rural areas. Zelzate has 12 700 inhabitants in total, approximately 1 470 (status of 9/10/2018, not including children) thereof live within 1 km radius to the plant.

The wastewater occurring at Rain Carbon is not subject to this application for authorisation since the whole formulation process is waterless (for more details see section 9.1.1.5). The drinking water for Zelzate comes from surface water sources which are located in at least 20 km distance from the plant.

9.1.1.4 Description of RMMs/OCs for workers:

Rain Carbon is certified with OHSAS 18001 (Occupational Health and Safety Assessment Series) and with ISO 9001 (Quality management and quality assurance standards) and 14001 (environmental management system).

Technical measures:

- The whole formulation process and loading of products is conducted in a closed system and via closed lines.
- All tanks and un-/loading stations for ships and tank trucks are equipped with exhaust air recovery/balancing systems on the top, which constantly draw and gather exhaust air.

- Exhaust air from the tanks and un-/loading stations is gathered and treated in a scrubber unit (see section 9.1.1.5).
- Pitch is pumped from the refinery to the pitch tank farm. The air displaced from the pitch tank farm is distributed in the total tank farm and thereby buffered, only accounting for a small volume of the overall air volume in the system. The pressure within the whole system increases only very slightly as the entire headspace of the tank farm acts as a buffer volume. Most ship operations are conducted under vapour return balancing, so no displacement volumes are introduced. Only barge unloading uses vapour recovery, with buffering in the tank farm and finally displaced volumes.
- The wet scrubbers are equipped with a valve (on the outlet to the atmosphere) that only opens when a pressure buildup in the tanks is registered, otherwise the system is fully closed.
- 90% of the pumps (including ship loading stations) are magnetically coupled and thereby have zero fugitive emissions (these pumps are equipped with an additional temperature sensor to detect possible heat generation at the magnets). The remaining 10% of pumps of other types will be replaced by magnetically coupled pumps in the next years.
- Closed sampling systems for tar oil and pitch are used at most sampling points (for a more detailed description of the closed sampling systems see section 9.1.3.2).
- Operators spend only the time necessary close to emission sources (segregation; e.g. during loading, after placing the loading arm, the truck driver retreats to his cabin, the operator to a local monitoring post.

Organisational measures:

- The furnaces are measured every month for combustion performance (e.g. O_2, CO, NO, NO_2, CO_2, SO_2). For the thermal incinerator, it is continuously monitored that the combustion temperature is sufficiently high in order to ensure the complete destruction of PAHs.
- New employees undergo a programme from the safety department at their start of work, which includes an extensive safety instruction, instructions on good occupational hygiene, waste, handling of carcinogenic substances, labelling and PPE. Every new employee is also checked by independent medical services for fitness.
- New employees also get environmental and quality introductions and training (e.g. how to use the systems that contain the instructions/procedures) by the Quality & SHE departments.
- New process operators and logistics operators are trained on the job by other experienced operators for three to six months.
- Workers participate in regular safety instructions via presentations of safety videos every two to three years.
- All workers are advised on the activities they are permitted to conduct assigned to their job matrix. They are instructed on all permits which are applicable, e.g. working

with combustible materials, suction works with vacuum pumps, high pressure cleaning, entering confined spaces, how lines have to be closed, etc.; a library of all permits is always accessible.

- The head of the each department tracks skills required vs skills mastered and records this in a competence matrix. This is a continuous process and serves as a basis to start training programs. Before a novice worker is allowed to work alone on a shift, all required skills have to be tested/acquired. Novice training starts with working during day shifts and the workers need to be able to operate independently when they are allowed to work during night shifts.
- A full instruction set is available to all employees (ISO 9001 / 14001 + OHSAS 18001 certified). All instructions are available digitally from any workstation and plant operators receive an individual paper copy. Written procedures for specific operations (e.g. how to open lines) are provided, close to the place of operation wherever possible (e.g. standard operating procedures at the fume hoods within the laboratory). Instructions are periodically reviewed / updated.
- MSDSs are presented to all workers and always available.
- A safety department is available on-site with five safety inspectors in shift, and three staff people in day service. All permits for routine and non-routine works are accessible at the safety department, wherein the PPEs for each operation are specified. For low risk works not requiring special permits outside of the standard work permit and securing installations permit, approval by the responsible engineer and control room of the production plant is sufficient.
- The PPE are organized and distributed by the safety department; a central storage with a reception centre is available and accessible at all times. Advice is provided to the workers on the appropriate equipment they need assigned to their job matrix. This is typically under the format of toolbox meetings and includes e.g. how to handle contaminated gloves and how to pull them out without contaminating hands.
- Permits for none-routine works are also available at the safety department and the workers are advised about what to wear.
- Advice is provided in the general safety instructions, through toolboxes and through personal advice by the safety inspectors
- The proper functioning of the PPE is regularly inspected and maintained by the safety inspector or external parties meeting at least the legal standards for periodicity. This covers e.g. integrity checks of chemical suits, full facial masks, functionality check of respiratory masks, field inspections for correct use of PPE's.
- The workers are provided with several sets of working clothes and encouraged to change them daily. The worn clothes are sent to an industrial cleaning service two times a week.
- Separate changing rooms are available for the workers with separate lockers for dirty and clean clothes. Bins are provided in front of the changing rooms that dirty clothes can be dropped.

- Shelves for helmets and gloves and a waste container for dirty gloves are provided in front of the control room.
- Disposal of waste for contaminated equipment is organized, in closed containers for all types of contaminated waste.
- Big signs are placed at each working station indicating which PPE has to be worn for the respective operation/product.
- Systems are in place that allow all employees to report unsafe situations, non-conformities and to suggest improvements in working conditions.
- Full emergency response is available on site 24/7.
- Initial medical check-up followed by regular medical check-up of all employees (three months – one year), with frequency depending on likelihood of potential exposure.
- Regular exposure measurement campaigns are conducted.

Personal protection:

- The PPEs are organized and distributed by the safety department. The workers are provided with the appropriate equipment they need assigned to their job matrix. PPEs (Working clothes [EN 13034], coveralls [EN 14605], gloves [EN 374], goggles [EN 166], face shields, and respiration masks [EN 405, EN 140, EN 136]) are used by the workers according to the tasks they perform.
- For pitch works: respiratory protection (full face mask with ABEK filter) has to be worn by the workers during all activities where a moment of exposure might be possible (e.g. for truck un-/loading, coupling and decoupling; when raw material is coming in and the loading cone is manoeuvred into the manhole or physically moved).
- The following gloves are worn by the relevant exposed groups:
    - Operators: Heavy duty SHOWA 720R nitrile gloves are worn as standard operator gloves for occasional contact.
        - A long sleeve version of the nitrile heavy duty glove is equally available
        - For high temperature works neoprene gloves with cotton jersey liner are used (Ansell Scorpio 09-022)
        - In case of anticipated more intense product contact Viton gloves are available.
    - Laboratory technicians: single use laboratory gloves (nitrile rubber) are worn
- For handling hot liquids (such as CTPht), a dedicated high temperature suit has to be worn to cover the risks of possible hot liquid spill.
- For lower exposure, filter masks can be worn; in case of higher exposure, a full face mask with breathing air supply independent of circulating air is worn.

- The site is visibly divided into zones (color-coded, defines the minimum level of PPE's to be worn at all times), dependent on the proximity of the installation and risks present in the surroundings.
- Ear protection is worn in the operational part of the plant (except in buildings), visitors are obliged to use earplugs.

Medical history of accidents with hot materials

OHS records show that in the past ten years, only two incidents with burns from hot pitch happened.

9.1.1.5 Description of RMMs/OCs for the environment:

Rain Carbon is certified ISO 14001 for Environmental management systems.

Emissions to water

The following precautions are taken by Rain Carbon in order to minimize the amount of water emissions:

- The whole formulation process is waterless.
- The water contained in the coal tar is separated in the tar refinery and sent offsite to a licensed waste water treatment company. This has no connection to uses of CTPht/AO that are subject to authorisation.
- The complete production and formulation area is paved. Rainwater from all surfaces and bunds of the plant is collected at specific points and led to an on-site water treatment plant (divided into a pre-treatment and a final stage).
- The total concrete surface of the plant is 35 200 m^2, of which 9 000 m^2 is the area of the pitch tank farm/pitch blending and 3 000 m^2 the area of the tank farm for oil blending.
- As formulation activities are rather static in fully closed tank farms, their contribution to rain water contamination is minor.
- Apart from the rainwater, the on-site water treatment plant also receives the water from the cleaning box, water used for technical applications and water from steam production and use. The amount of water arising from the cleaning of parts related to the formulation process is negligible.
- Sanitary water generated in the shower rooms and office toilets is the only stream that goes to the public sewer and WWTP.
- During shutdowns of the tar refinery an additional water treatment is rented (filtration + active carbon adsorption) to treat the water from the surfaces used for storing/cleaning the equipment before it runs to the final WWTP.
- Spillages are solidified, collected and discharged as solid waste

Specifications on rainwater treatment

- There are two WWTP's on-site:
    - WWTP 1: Dedicated to the process surface of the tar refinery, incl. cleaning box. The effluent of this goes to WWTP 2.
    - WWTP 2: Treatment plant for the entire concrete surface of the plant.
- Both plants use the same principle as explained below. The effluent of WWTP 1 has an additional active carbon adsorbent before going to WWTP 2
- General principle of the WWTP's:
    - Collection and decantation of the waste water (basin of 45.6 x 8.6 x 3 m in WWTP 2).
    - Addition of coagulant, followed by filtration over dynamic sand filters. Continuous monitoring of turbidity on both WWTP 1 and 2.
    - Adsorption of hydrocarbons on porous styrene-divinylbenzene resins. Continuous monitoring of phenols in influent and effluent of the resin beds in WWTP 2.
    - No biological treatment, thus no biosludge occurs.
- All coagulants, used resins and sedimented solid particles are sent as hazardous waste for incineration to an external company.
- The water of WWTP 2 is discharged in the canal, with continuous monitoring of flow and pH.
- Apart from the online analysis, samples are taken of WWTP 1 and 2 for lab analysis of BTEX, PAH, COD, BOD, etc.
- The wastewater treatment system has been audited by VITO (Vlaamse Instelling voor Technologisch Onderzoek) and has been confirmed as BAT for the water quality at the site (2010).

Emission to air

The following precautions are taken by Rain Carbon in order to minimize the amount of air emissions:

- The whole formulation process of CTPht and AO is conducted in closed equipment with 90% magnetic pumps for zero emission.
- All tanks and loading stations for trucks and ships are equipped with vapour return/balancing systems.
- The pitch tank farm for formulation of CTPht is closed and the vapour phase is interconnected between all tanks. The vapour lines are connected to the atmosphere via two wet scrubbers (waterless; runs with wash oil). The scrubber outlets is equipped with a valve that only opens in case the tank farm reaches a pressure of 1-3 mbar. This allows for buffering of most liquid transfer without emission to air: One scrubber is closed for 73%, the second scrubber for 23% of the time. The scrubbers

are countercurrent; the scrubber liquid is exchanged regularly and recycled in the tar refinery. During 2019, these two scrubbers will be extended with an activated carbon adsorbent in order to reduce the emission to even lower levels.

- The oil tank farm for formulation of AO has an equivalent interconnected vapour phase and scrubber system (scrubbers are waterless; run with wash oil). During 2019, the scrubber outlet will be connected to the incinerator of the tar refinery.
- Flue gases of all furnaces (incl. the thermal incinerator of the tar refinery) are analyzed monthly. The combustion temperature of the incinerator is measured and controlled online for complete combustion of PAHs.
- During demolition/cleaning of tanks, a case-specific emission control system is used. (e.g. forced draft + filtration/active carbon adsorption). As these operations are very rare (tank lifetime >30 y), the relevance for the exposure assessment is very low.

Fugitive emissions – mass balance considerations

There are specific measures in place to survey the whole plant regularly and continuously for fugitive emissions. Due to the physico-chemical properties of 3- to 5-ringed PAHs, fugitive emissions are not considered a critical point for these substances, but the measures listed below are guaranteeing also to detect minor emission sources for PAHs. In case of leakages CTPht would rapidly cool down, reducing further the vapour pressure of contained PAHs. Leakages are easily detectable due to the deep black colour of all pitch-containing materials and would be noticed immediately by the surveys regularly conducted by operators.

Mass balances are difficult to establish for PAHs. Mass balance calculations for CTPht and AO essentially show that all the material produced by tar distillation leaves the plant in form of the various products (either neat or mixtures) (minus the small quantities of solid waste as described below). However, due to the large quantity of products and the low concentration of PAHs in the products, no further quantification is possible.

General measures to control and reduce fugitive emissions at the site:

- A source reduction program is performed by Rain Carbon which includes for instance yearly check-ups for leak detection (LDAR = leak detection and repair, ±7 000 points measured every year) by an external company (in order to decrease benzene emissions continuously).
- Monitoring data on fugitive emissions of benzene are available; emissions coming from formulation process are not expected due to the closed system.
- In the framework of the ISO 14001 environmental management system, complaints (e.g. smell, noise, visual) from third parties are logged. Root cause analysis, corrective and preventive measures are run and documented.
- Volatile organic compounds (VOC) are continuously measured; 100 measurement points are distributed at all points on the plant where fugitive emissions may arise; an alarm system is installed which alerts if fugitive emissions above 10 (warning) and 15 (high alert) ppm are detectable.
- Ship loading is monitored for fugitive emissions. Pressure which might build on the ship by wrong settings during loading could lead to fugitive emission (= smell) if it is

not counteracted. Rain Carbon installs wireless pressure measurements on board of the ship (connected to the plant´s Distributed Control System (DCS)) in order to be proactive and to control the ship. In case that excess pressure builds up, the loading is stopped (simple measure which could otherwise result in emission; no smell arises due to this proactive measure).

- The sampling systems for tar and tar oils (incl. AO) are already fully closed, using dedicated sampling valves and container. For CTPht, the sampling points are equipped with local ventilation and cleaning of the extracted air on an active carbon adsorbent. By Q2 2019 all CTPht sampling points will be equipped with this system. For a more detailed description of the closed sampling system for pitch mixtures see section 9.1.3.2).
- Benzene is measured at several stations in Flanders (operated by the Flemish environmental agency); one station is in the direct surroundings of the plant and of Zelzate. The monitoring data are publicly available. This station is at 150 m distance to the plant in the dominant wind direction, benzene is still measured at this station but PAH measurements were stopped in 2014/2015 since the emission values were always comparable to those from another station 1.7 km away (between a steel plant and Rain Carbon. Several campaigns are running, all data are collected, reports are publicly available.

9.1.1.6 Handling of waste

- Waste from formulation processes originates only in very low quantities at the plant of Rain Carbon:
    - Contaminated protective equipment (e.g. gloves) and materials
    - Samples containing CTPht and/or AO
    - Liquid waste from the rare spillages or leakages (occur rather from the general production process and not from formulation as the amount of valves/operations in production is much higher. If any, the amount of spillages or leakages from the formulation process is solidified with sand, soil and adsorbents)
- Every waste which might be CTPht/AO-contaminated is gathered on-site in closed containers and sent as hazardous waste for incineration to an external company. The external company is licensed for destruction of hazardous waste; their process is incineration in rotary kilns with heat recuperation and flue gas cleaning.
- Active carbon filters (from the air treatment at the pitch sampling stations) are changed every six months and the used active carbon can be either sent for thermal regeneration or sent out with the standard hazardous waste.

9.1.1.7 Description of technical improvements achieved and planned:

Measures of Rain Carbon to reduce emissions and exposures of the Annex XIV substances in recent years and in the future are listed below.

List of improvements:

- The sampling systems for mixtures containing CTPht and/or AO are already fully closed, using dedicated sampling valves and container. For CTPht the sampling points are equipped with local ventilation and cleaning of the extracted air on an active carbon adsorbent. By Q2 2019 all CTPht sampling points will be equipped with this system. For a more detailed description of the closed sampling system for pitch mixtures see section 9.1.3.2).
- A step-wise decrease of the emissions of the 16 EPA PAHs via rainwater release is fixed in the environmental license of Rain Carbon (in three levels from 2011 to 2019; see official release permits for water in Annex II.) A source reduction program has been executed since 2009 and still is running today on the entire site, resulting in the continuous decrease of PAH in water/air emissions.
- In the framework of this source reduction program, a new equipment cleaning box is planned for 2019; a closed building with a more user-friendly material-setup, integrated dedicated water treatment, continuous air extraction and treatment by adsorption.
- All tanks are continuously monitored and continuously renewed where necessary (based on an extensive preventive inspection program). Steel tanks are replaced by stainless steel tanks where this provides advantages. This inspection program contributes to prevent emissions from the tanks. All tanks are either in a bund or have a double-wall construction.
- The main power supply line to the plant was recently renewed (dual cable for full redundancy) in order to prevent shutdowns due to electrical power outages (unforeseen shutdowns constitute higher risks for emissions). Also the high voltage equipment on the plant has been renewed.

9.1.2 Environmental contributing scenario 1

9.1.2.1 Conditions of use

Table 9-12: Conditions of use

Amount used, frequency and duration of use (or from service life)
• Annual use amount at site: [redacted] (0-300 000) tonnes CTPht/year and [redacted] (10 000-50 000) tonnes AO/year
Technical and organisational risk management measures
• Formulation processes are conducted in a closed system and via closed lines • Exhaust gases are collected from all tanks and loading stations and sent to scrubbers
Conditions and measures related to wastewater treatment
• Formulations are produced without water • Onsite treatment of rainwater: physical separation (decantation, addition of coagulant, filtration over dynamic sand filters), adsorption of hydrocarbons on porous styrene-divinylbenzene resins, active carbon adsorbents • Application of STP sludge on agricultural soil: No sludge occurs since the rainwater is not led to an STP with biological treatment • Discharge rate: 303 m^3/day (mean daily discharge rate for the years 2012-2018; total discharge rate to canal) from WWTP 2
Conditions and measures related to external treatment of waste (including article waste)
• Particular considerations on the waste treatment operations: liquid and solid waste is collected by an external company certified to collect hazardous waste and is incinerated by an authorised company according to national legislation
Other conditions affecting environmental exposure
• Receiving surface water flow rate: 1 123 200 m^3/day (= 13 m^3/sec; minimal flow rate of the canal "Zeekanaal Gent-Terneuzen")

9.1.2.2 Releases

Table 9-13: Local releases to the environment

Release	Release rate estimation method	Explanation / Justification
Water	Measured	Local release rate: 157 mg/day (mean daily release rate for the years 2012-2018; sum of 9 PAHs relevant for the PBT assessment of CTPht and AO, for individual substances see Table 9-15) Explanation / Justification: measured data

Release	Release rate estimation method	Explanation / Justification
Air	Measured	Local release rate: 2.56 g/day (sum of 9 PAHs relevant for the PBT assessment of CTPht and AO, for individual substances see Table 9-14) Explanation / Justification: measured data
Soil	-	Final release factor: 0% Explanation / Justification: no emission to soil

Releases to waste

The amount of waste arising from formulation activities at Rain Carbon is negligible. Only solid waste is produced in small quantities (e.g. samples; estimate: 50 kg/year); larger quantities are very rare (e.g. tank cleaning for inspection). All waste is incinerated by an external service provider and therefore no release has to be considered.

Release factor to waste from the process: 0

Release factor to waste from on-site treatment: 0

9.1.2.3 Exposure for the environment

Description of data used for the assessment of environmental exposure and for exposure assessment of humans via the environment:

Emissions to air

PAH air emissions relevant for this AfA come from four different scrubbers: two scrubbers from the pitch storage park (scrubbers K101 and K102), one scrubber from the storage park for tar oils (scrubber K100A) and one scrubber for oils and pitch combined (31B101). Note for the storage park for tar oils that the tanks dedicated to storage of AO (= AO low; which is the AO subject to this AfA) only account for 66.1% of the park and the total PAH emission from scrubber K100A overestimates the emission coming from AO formulations by 33%.

Given that the transfers of large volumes at high flowrates on the site are equipped with vapour return/balancing systems, the scrubbers operate in steady conditions.

Emission data to air are available for the ten PAHs relevant for this AfA (nine PAHs relevant for the environmental assessment, see Table 9-3 in section 9.0.3.1; four PAHs relevant for oral exposure of humans via the environment, see section 9.0.3.2) for the years 2009, 2012 and 2018 (raw data provided in Annex III). The emission calculations are based on measured PAH concentrations. Air from the scrubber chimney is extracted and adsorbed on XAD® resins. The adsorbent is then desorbed in the laboratory and GC-MS analysis yields the PAH concentrations. Details on detection limits are provided in Annex III.

There is some variation in the emission of PAHs per scrubber and per year (see Annex III). The low flowrates of the scrubbers are often below the minimum flow of the flowrate instruments. For the 2018 calculation of the total quantity emitted, average flowrates from all 2018 measurements and process data have been used.

The related uncertainty is considered in an uncertainty analysis discussed in chapter 9.1.2.4. Note that emission rates for the 9 PBT substances were higher in 2009 compared to 2018, whereas the emissions of the 4 EFSA PAHs used for the assessment of exposure of humans via the environment were higher in 2018.

From the measurements conducted in 2009 and 2012, the higher emission values were selected for a conservative environmental assessment. The total emission from all four scrubbers was higher by a factor of 30 in 2009 than in 2012 for the sum of 9 PAHs relevant for PBT assessment. For the sum of 4 EFSA PAHs relevant for the assessment of HvE, the total emission was lower by a factor of 3.8 in 2009 than in 2012. Since the factor for the PBT substances was much higher than the factor for the 4 EFSA PAHs, usage of the data set from 2009 for the environmental assessment was considered the most conservative approach.

By end of 2019, the scrubbers K101, K102 and 31B101 will be post-treated on activated carbon (for details on the efficiency of PAH adsorption on activated carbon see Annex IV) and scrubber K100A will be connected to the thermal incinerator of the tar refinery (a temperature of 850-890°C and a residence time of 2 seconds ensures complete destruction of PAHs). From these technical improvements, emission reduction yields of >80% for K101, K102 and 31B101 and of 99-100% for K100A are expected in the future. Accordingly, for the environmental assessment of PAH emissions to air for 2020 onwards, reduction factors of 80% for the scrubbers K101, K102 and 31B101 and of 99% for scrubber K100A were applied on the emission data from 2009 (for comparison of 2009 emissions with and without applied reduction factors see Annex V). The resulting PAH emissions are shown in Table 9-14.

Table 9-14: PAH emissions to air from scrubbers K101, K102, K100A and 31B101 in 2009 [kg/year] with applied reduction factors due to technical improvements installed from end of 2019 onwards

Scrubber	K101	K102	K100A	31B101	Sum of all 4 scrubbers
	Emission [a] reduced by 80% [b]	Emission [a] reduced by 80% [b]	Emission [a] reduced by 99% [c]	Emission [a] reduced by 80% [b]	Reduced emissions
Anthracene	2.60E-03	8.00E-06	4.50E-07	1.16E-01	1.18E-01
Phenanthrene	2.60E-03	9.00E-04	7.90E-04	6.38E-01	6.42E-01
Fluoranthene	8.00E-06	9.00E-04	9.00E-05	1.16E-01	1.17E-01
Pyrene	8.00E-06	8.00E-06	4.50E-07	5.78E-02	5.78E-02
Benzo[a]anthracene	8.00E-06	8.00E-06	4.50E-07	8.00E-06	2.45E-05
Chrysene	8.00E-06	8.00E-06	4.50E-07	8.00E-06	2.45E-05
Benzo[a]pyrene	8.00E-06	8.00E-06	4.50E-07	8.00E-06	2.45E-05
Benzo[b]fluoranthene [d]	8.00E-06	8.00E-06	4.50E-07	8.00E-06	2.45E-05
Benzo[k]fluoranthene	8.00E-06	8.00E-06	4.50E-07	8.00E-06	2.45E-05

Benzo[ghi]perylene	8.00E-06	9.00E-04	4.50E-07	8.00E-06	9.16E-04
9 PAHs relevant for PBT assessment	5.26E-03	2.75E-03	8.83E-04	9.27E-01	9.36E-01

[a] In case that the emission was provided with "<" in the raw data table (see table above), the given value was divided by 2 (considering LOD/2 for the measured concentration).

[b] A conservative reduction of 80% was applied to the emission value since emission from this scrubber will be post-treated on activated carbon from end of 2019 onwards and a yield of 80-99% removal is expected.

[c] A conservative reduction of 99% was applied to the emission value since emission from this scrubber will be post-treated on activated carbon from end of 2019 onwards and a yield of 99-100% removal is expected.

[d] Not PBT; environmental modelling performed as substance is required for calculating the sum of 4 EFSA PAHs for the assessment of HvE.

Further emissions to air via volatilization from surface waters (or e.g. the rainwater collection basin on the plant) are considered insignificant under field conditions due to the low vapour pressures of the ten PAHs (in the range of 10^{-2}-10^{-10} Pa; see Table 9-4 in section 9.0.3.1), as described in section 4.2.2 (ECHA, 2009c; The Netherlands, 2008).

Emission to water

The water coming from the on-site WWTP 2 (gathering rainwater from the whole plant, water from the cleaning box, water used for technical applications and water from steam production and use) is sampled within the scope of a regular monitoring programme conducted at Rain Carbon before it is released into the canal. The point where the treated water coming from WWTP 2 is sampled (by a continuous automated sampler) and introduced into the canal is indicated (as a red dot) on the site map shown in Figure 9-1.

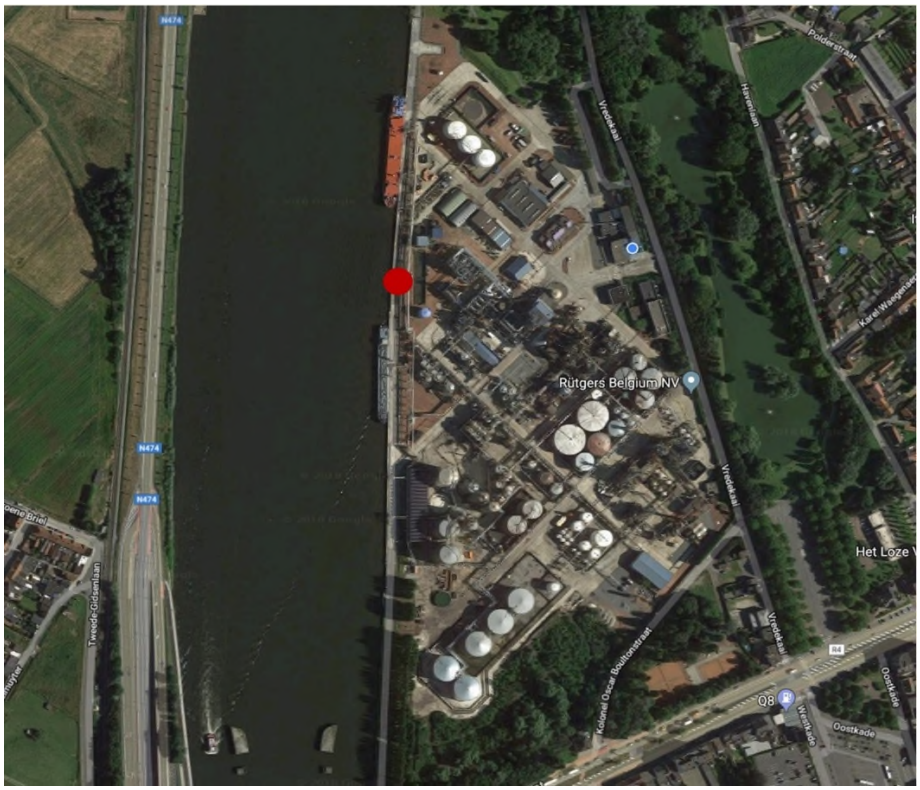

Figure 9-1: Indication of release point

Several parameters were measured regularly in these samples between 2001 and 2018, including the concentrations of the ten relevant PAHs (in 2018: 62 measurements until July; in 2017: 99 measurements in total; for the years before 2017: typically 52-100 samples per year).

From the measured concentrations and the total discharge volumes of water from WWTP 2 into the canal, the PAH emissions for 2001-2018 were calculated (for emission data and discharge volumes for all years see Annex VI). These data show that the PAH emissions decreased continuously over the years, being the result of the step-wise source reduction program running on the entire site (reduction of sources, contaminated equipment renewed/replaced). Through these measures, Rain Carbon has been able to follow the stepwise reduction in the environmental permit. The internal PAH reduction program is still ongoing and aims for a continuous improvement in emission characteristics to both air and water.

Since the most prominent decrease (approximately by factor 7) of PAH emissions is visible from 2012 onwards, data for 2012-2018 are considered representative for the current PAH emissions into the canal. As shown in

Table 9-15, the highest emissions within these years occurred in 2016, which can possibly be explained by a high amount of sediments in the basin at the entrance of the WWTP in this year. (The basin has been cleaned and collected sediment has been sent to licensed hazardous waste incineration.) With these slight variations in PAH emissions per year, the usage of mean values for 2012-2018 was considered most appropriate for realistic environmental exposure calculations.

Table 9-15: Total PAH emissions to water and discharge volumes from WWTP 2 per year (2012-2018)

Emission [mg/day]								
PAHs	2012	2013	2014	2015	2016	2017	2018	Mean 2012-2018
Anthracene	47.1	32.8	3.5	10.6	11.6	18.0	16.8	19.9
Phenanthrene	17.8	16.8	12.8	16.2	31.9	65.0	68.7	33.2
Fluoranthene	22.6	21.2	8.3	13.6	95.7	53.2	55.1	39.7
Pyrene	11.5	12.5	4.1	6.6	61.8	29.6	25.8	22.4
Benzo[a]anthracene	2.0	7.5	2.2	1.4	20.0	11.9	15.2	8.8
Chrysene	2.5	5.4	6.7	2.1	22.4	19.9	18.9	11.3
Benzo[a]pyrene	3.6	7.0	3.8	1.3	16.1	16.4	11.1	8.6
Benzo[b]fluoranthene [a]	2.3	8.3	5.1	2.3	32.8	31.8	23.4	15.5
Benzo[k]fluoranthene	1.9	5.6	2.6	2.1	12.0	13.0	12.6	7.2
Benzo[ghi]perylene	0.9	2.1	0.6	1.0	11.0	13.6	10.2	5.8

9 PAHs relevant for PBT assessment	110.5	113.0	45.2	55.9	293.5	254.2	244.6	156.9
Discharge volume [m^3/year]	111 206	122 377	118 242	101 183	101 231	109 413	109 413 [b]	110 438
Discharge volume [m^3/day]	305	335	324	277	277	300	300 [b]	303

Unrounded values used for calculation.

[a] Not PBT; environmental modelling performed as substance is required for calculating the sum of 4 EFSA PAHs for the assessment of HvE.

[b] Value is estimated based on the discharge volume from 2017.

The pre-treated rainwater from the outlet of WWTP 2 is led via a short pipe (approximately 15 m) into the canal "Zeekanaal Gent-Terneuzen". The canal´s flow rate is – amongst other factors such as tidal effects – a result of human manipulations and therefore, its water drainage function is subject to very large variations which make it difficult to capture a fixed or static flow rate. However, a minimal flow rate of 1 123 200 m^3/day (= 13 m^3/sec) could be estimated, which is used to calculate the dilution factor of the rainwater discharged into the canal (more information on the flowrate is provided in the report "*Project – MER, Hervergunning en uitbreiding PR0429"* [1]. The minimum flowrate for the canal has been set in a treaty between Belgium and the Netherlands.

Approach to EUSES modelling

EUSES modelling was performed for air emissions from formulation activities (Table 9-14) and water emissions from WWTP 2 into the canal (Table 9-15).

The general information provided for the twelve indicator PAHs in section 9.0.3.1 was used for EUSES calculations.

Furthermore, the following site-specific parameters were applied for the assessment of environmental exposure and of exposure of humans via the environment:

- For the local release fractions (direct emissions from formulation activities at the plant), the emissions into the canal were considered in EUSES as *emissions to wastewater* bypassing an STP (instead of *emissions to surface water*) in order to adapt discharge and canal flow information. The *fractions of tonnage released to surface water and industrial/agricultural soil* were set to 0 (according to Table 9-13).
- The local *fraction of tonnage released to wastewater* was calculated by dividing the water emissions from on-site WWTP 2 into the canal (e.g. [g/day]; as provided above in Table 9-15) by the "*production volume of chemical in EU*" (e.g. [g/day]) for each individual PAH. The *production volumes* of the individual PAHs were obtained as follows:

[1] *Project – MER, Hervergunning en uitbreiding PR0429;* https://www.milieuinfo.be/dms/d/d/workspace/SpacesStore/4a284860-daf6-417e-b162-45ab1fd94401/TEC0811007SVdB_Rutgers_MER_ev_2.pdf

- CTPht: multiplying the tonnage information for CTPht in special tars (see Table 9-10) with the concentration of PAHs according to the composition of CTPht in the European Composite Sample as indicated in Table 1-3
- AO: multiplying the tonnage information for AO in CBF (see Table 9-11) with the concentration of PAHs according to the composition of AO in the European Composite Sample as indicated in Table 1-4
- The *production volumes* of PAHs coming from formulations with CTPht or AO were summed up for each individual PAH

Note that the calculation of release fractions is an entirely technical issue, since the releases from WWTP 2 are based on measured data.

- The emission scenario "bypass STP" was considered most appropriate for EUSES modelling of the environmental emissions. Although water released into the canal is pre-treated on the plant (via decantation, adding coagulants, filtration, adsorption on styrene-divinylbenzene resins), no biological treatment is conducted on-site. Accordingly:
  - emissions of PAHs to air via volatilization are considered negligible during this pre-treatment procedure, due to the low vapour pressures and Henry´s Law constants of the PAHs (see Table 9-4), as described in section 4.2.2. This is also mirrored in the modelled distribution of PAHs in an STP with activated sludge treatment, where 0% emission of benzo[a]pyrene into the air can be expected (see Table 4-6).
  - no biosludge occurs and emissions to soil or grassland via sludge are non-existent
- The regional exposure scenario was synchronized with the local scenario since only one site (the local assessment) is relevant for environmental exposure modelling in EUSES. Per default in EUSES, the local release to wastewater (= *production volume of chemical in EU* x *fraction of tonnage released to wastewater*) is identical with the *regional release to wastewater* but the *regional release to wastewater* is split into two fractions for the regional assessment: 80% are considered as *total regional emission to wastewater* and 20% as *total regional emission to surface water*. Since no "real" release to wastewater is present in the local scenario (*emissions to wastewater* bypassing an STP, as described above), the release fractions on the regional scale were adjusted accordingly: 0% (instead of 80%) as *total regional emission to wastewater* and 100% (instead of 20%) as *total regional emission to surface water*. For the *regional release to air and industrial/agricultural soil*, EUSES uses per default the same tonnage fraction as on the local scale and no adjustment was necessary.

  Note that these adaptations are required to reflect the fact that only emissions from a single site have to be considered in this assessment. Since the local and the regional assessments in EUSES are not coupled (i.e. local emissions are not 'diluted' in the regional environment), the adaptations are necessary to reflect regional concentrations resulting from local emissions.
- The *number of emission days per year* is 365.

- The canal as receiving water was considered as a "river" in EUSES (the Westerschelde estuary is approximately 15 km distant to the release point and thereby the salinity of the canal is increased (0.4-0.75%, brackish water; for details on salinity see Annex VII), and the distribution zone in the canal is cone-shaped until it reaches the estuary).
- A dilution factor of 1 000 was applied for the water emissions into the canal, although the actual dilution factor would be 3 712 (1 123 200 m^3/day /303 m^3/day = 3 712; as described above). However, in agreement with the Guidance on Information Requirements and Chemical Safety Assessment Chapter R.16: Environmental exposure assessment (version 3.0), "*a dilution factor higher than 1 000 should not be used in any case, since the concentration in the mixing zone can be higher than the concentration estimated by a complete mixing of the effluent and the mixing zone can be very large for high dilution factors (see Appendix A.16-3.3.3)*" (ECHA, 2016).
- Due to the very conservative nature of the EUSES modelling of the oral uptake via food, more adequate food consumption data were used instead of the EUSES defaults. Based on a representative survey on Belgian food consumption from the Scientific Institute of Public Health (WIV-ISP) in Brussels (National Food Consumption Survey 2014-2015[2]), the default values for consume of the five food categories considered in EUSES (root crops, leaf crops, dairy products, meat and fish) were adapted to the Belgian population. The composition and consumed amounts of these five food categories are provided in Annex VIII, comparing the EUSES defaults with the numbers from the survey (in cases where a food category consists of more than one group considered in the survey, the sum of all groups was calculated). The defaults were replaced in EUSES by the mean value calculated for each of these categories (bold numbers), as the mean values are considered to represent best the life-long food consumption behaviour.

The EUSES protocols for the assessment of the ten PAHs are provided in Annex IX.

The following Table 9-16 shows the total PAH emissions and their relative distribution to water and to air. These emission data are based on the measurements shown above. Note that the emissions to water are further distributed to the sediment.

Table 9-16: PAH emission distribution to water and air

	Emissions (surface water and air)		**Emission to surface water**		**Emission to air**	
	[kg/year]	[%]	[kg/year]	[%]	[kg/year]	[%]
Anthracene	1.25E-01	100	7.25E-03	5.78	1.18E-01	94.22
Phenanthrene	6.54E-01	100	1.21E-02	1.85	6.42E-01	98.15

[2] National Food Consumption Survey 2014-2015;

https://fcs.wiv-isp.be/nl/Gedeelde%20%20documenten/FRANS/Rapport%204/Rapport_4_FR_finaal.pdf

Fluoranthene	1.31E-01	100	1.45E-02	11.05	1.17E-01	88.95
Pyrene	6.60E-02	100	8.19E-03	12.41	5.78E-02	87.59
Benz[a]anthracene	3.23E-03	100	3.21E-03	99.24	2.45E-05	0.76
Chrysene	4.16E-03	100	4.14E-03	99.41	2.45E-05	0.59
Benzo[a]pyrene	3.16E-03	100	3.13E-03	99.23	2.45E-05	0.77
Benzo[b]fluoranthene *	5.68E-03	100	5.66E-03	99.57	2.45E-05	0.43
Benzo[k]fluoranthene	2.67E-03	100	2.64E-03	99.08	2.45E-05	0.92
Benzo[ghi]perylene	3.02E-03	100	2.11E-03	69.67	9.16E-04	30.33
Sum of 9 PBT PAHs relevant for the PBT assessment	9.93E-01		5.73E-02		9.36E-01	
* Not PBT; environmental modelling performed as substance is required for calculating the sum of 4 EFSA PAHs for the assessment of HvE.						

EUSES output data

Water, sediment and soil

The Predicted local Environmental Concentrations (local PECs), which were obtained from EUSES modelling for diverse compartments, and the respective Predicted No Effect Concentrations (PNECs) are shown in Table 9-17.

Table 9-17: Local PECs (calculated by EUSES) for diverse compartments compared with the PNECs (from Table 7-4)

	PEC local			PNEC		
	PEC fresh water [mg/L]	PEC fresh sediment [mg/kgdwt]	PEC soil [mg/kgdwt]	PNEC fresh water [mg/L]	PNEC fresh sediment [mg/kgdwt]	PNEC soil [mg/kgdwt]
Anthracene	6.31E-08	1.86E-04	1.60E-06	1.00E-04	1.40E-01	1.26E-01
Phenanthrene	1.06E-07	2.44E-04	8.50E-06	1.30E-03	5.00E+00	1.80E+00
Fluoranthene	1.15E-07	1.12E-03	2.32E-06	1.00E-05	9.60E-01	1.50E+00
Pyrene	6.82E-08	4.02E-04	9.12E-07	2.30E-05	2.80E+00	1.00E+00
Benz[a]anthracene	1.66E-08	8.33E-04	4.80E-09	1.20E-05	6.01E-01	7.90E-02
Chrysene	2.35E-08	9.35E-04	5.84E-09	7.00E-05	2.79E+00	5.57E-01
Benzo[a]pyrene	1.27E-08	1.05E-03	8.54E-09	2.20E-05	1.83E+00	5.30E-02
Benzo[k]fluoranthene	1.09E-08	8.69E-04	8.52E-09	1.70E-05	1.35E+00	2.70E-01
Benzo[ghi]perylene	7.57E-09	7.72E-04	3.16E-07	8.20E-06	8.36E-01	1.67E-01

Although it is not the aim of this AfA to follow a threshold approach for PBT substances, Risk Characterisation Ratios (RCRs) are calculated to visualize the differences between PECs and no effect concentrations.

The comparison of these data shows that the PECs of all compartments are at least two orders of magnitude lower than the respective PNECs. Accordingly, the local RCRs, which are obtained by dividing the local PEC by the PNEC for each compartment, indicate a very low (<<1) risk for environmental effects (Table 9-18).

Table 9-18: Local RCRs for diverse compartments as calculated by EUSES

	RCR fresh water	RCR fresh sediment	RCR soil
Anthracene	6.31E-04	6.65E-04	1.27E-05
Phenanthrene	8.18E-05	2.44E-05	4.72E-06
Fluoranthene	1.15E-02	5.84E-04	1.55E-06
Pyrene	2.97E-03	7.18E-05	9.12E-07
Benz[a]anthracene	1.38E-03	1.38E-02 *	6.08E-08
Chrysene	3.36E-04	3.36E-03 *	1.05E-07 *
Benzo[a]pyrene	5.75E-04	5.75E-03 *	1.61E-07
Benzo[k]fluoranthene	6.44E-04	6.44E-03 *	3.16E-07 *
Benzo[ghi]perylene	9.23E-04	9.23E-03 *	1.89E-05 *

* The equilibrium partitioning method was used to calculate the PNEC and an extra assessment factor of 10 was applied to the PEC/PNEC ratio in EUSES (in all cases the PAH has a log K_{OW} >5), leading to a 10-fold increase of the RCR.

Beside the low RCRs, also the comparison of local PEC values in freshwater with the Environmental Quality Standards in inland surface waters (EU, 2013), available for anthracene, fluoranthene and benzo[a]pyrene, shows that the water emissions from Rain Carbon have a negligible impact on environmental organisms. The calculated $PEC_{freshwater, bulk}$ values of the individual PAHs are between one and four orders of magnitude lower than the Environmental Quality Standard for inland surface waters (Table 9-19). Accordingly, the predicted environmental PAH concentrations resulting from Rain Carbon´s emissions are much lower than the Environmental Quality Standard concentrations in inland surface waters concentrations as defined by the European Commission (EU, 2013).

Table 9-19: Comparison of $PEC_{freshwater,\ bulk}$ values with Environmental Quality Standards for inland surface waters

	PEC freshwater, bulk [a] [mg/L]	Environmental Quality Standard AA-EQS [b] in inland surface waters [c] [mg/L]	Ratio
Anthracene	6.76E-08	1.00E-04	6.76E-04
Phenanthrene	1.12E-07	-	
Fluoranthene	1.42E-07	6.30E-06	2.26E-02
Pyrene	7.80E-08	-	
Benz[a]anthracene	3.68E-08	-	
Chrysene	4.63E-08	-	
Benzo[a]pyrene	3.84E-08	1.70E-07	2.26E-01
Benzo[k]fluoranthene	3.20E-08	[d]	
Benzo[ghi]perylene	2.64E-08	[d]	

[a] The PEC freshwater bulk was calculated from the PEC freshwater for comparison with the Environmental Quality Standards.

[b] This parameter is the EQS expressed as annual average value (AA-EQS). Unless otherwise specified, it applies to the total concentration of all isomers (EU, 2013).

[c] Inland surface waters encompass rivers and lakes and related artificial or heavily modified water bodies (EU, 2013).

[d] For the group of priority substances of PAHs, the biota EQS and corresponding AA-EQS in water refer to the concentration of benzo[a]pyrene, on the toxicity of which they are based. Benzo[a]pyrene can be considered as a marker for the other PAHs, hence only benzo[a]pyrene needs to be monitored for comparison with the biota EQS or the corresponding AA-EQS in water (EU, 2013).

In order to assess the impact of the water emissions from the plant on the aquatic environment close to the release point, the PEC values were also compared with publicly available data on PAH concentrations found in the canal "Zeekanaal Gent-Terneuzen" at the measuring point MP 30000 (Long.: 3.8031; Lat.: 51.2076; shown in Figure 9-2), approximately 200 m downstream of the emission point (which is also affected by other emission sources located close to Rain Carbon, upstream of the canal). The PAH concentrations measured in surface water (reported between 1991 and 2013) and in sediment (reported between 2002 and 2012) (database "Waterbase TCM" via the Information Platform for Chemical Monitoring (IPChem)[3]) were used for comparison with the calculated local PECs.

[3] Information Platform for Chemical Monitoring; https://ipchem.jrc.ec.europa.eu/RDSIdiscovery/ipchem/search_viewer.html; accessed on 23th November 2018

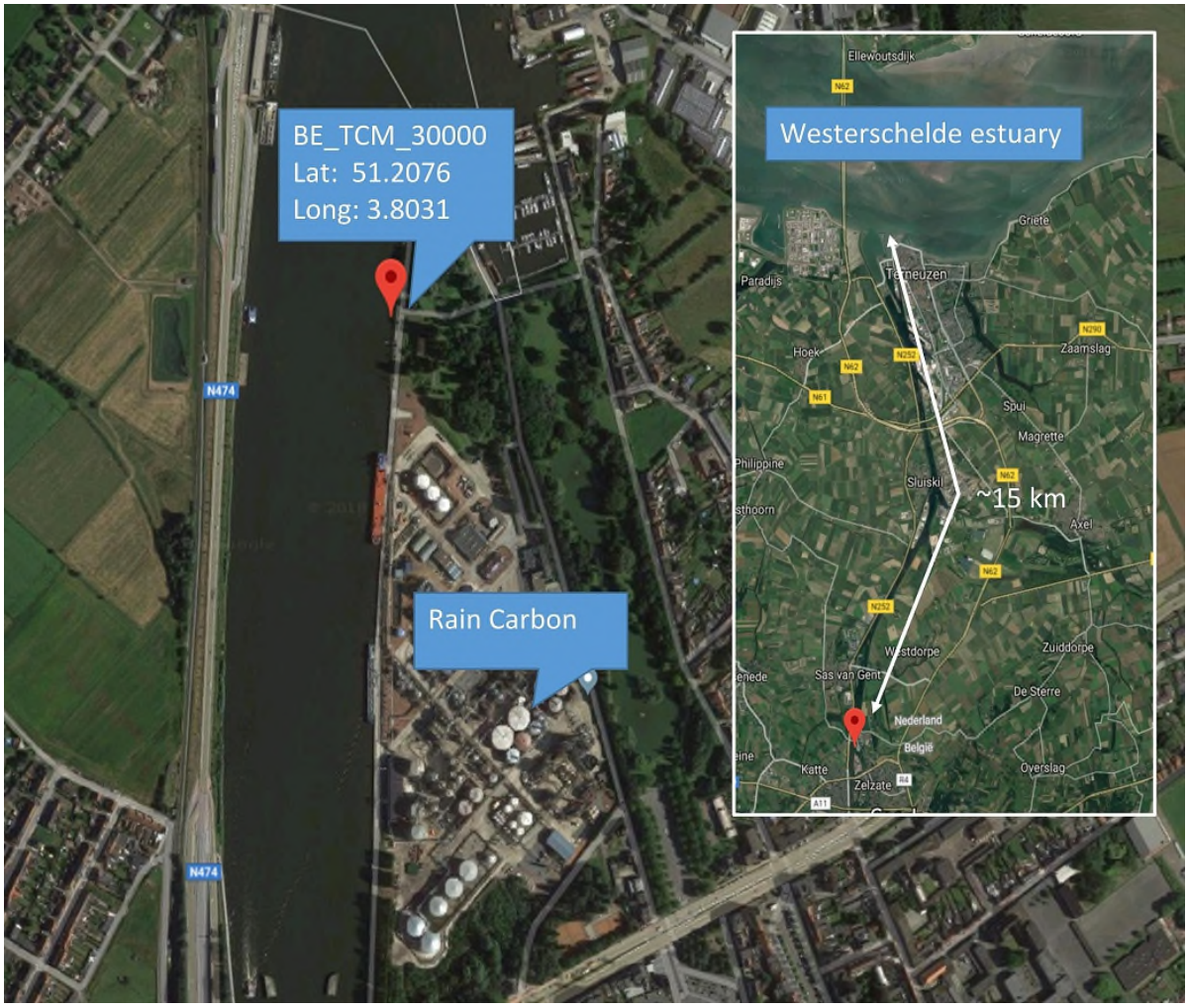

Figure 9-2: Location of the measuring point MP 30000 in the canal "Zeekanaal Gent-Terneuzen"

Although the environmental sample matrices are shown as "marine water" and "marine sediment" in the "Waterbase TCM" database, they are compared with PECs for freshwater and freshwater sediment, since the water in the canal is actually fresh water with an increased salt content due to the influence of tidal water ("brackish water", see Annex VII) and release and distribution into a freshwater compartment (i.e. a "river") was assumed for EUSES modelling (as described above for the EUSES input parameters).

As shown in Table 9-20, the PECs in freshwater are between two and five orders of magnitude lower than the mean and the maximum concentration measured in the surface water of the canal water at MP 30000 during the indicated period. The PECs in freshwater sediment are three to five orders of magnitude lower than the mean and the maximum of the measured concentrations for canal sediment at this point during the indicated period.

The "Zeekanaal Gent-Terneuzen" is subject to numerous PAH emission sources upstream of the measuring point, including industry (coal, oil, steel, chemicals), population, traffic and transportation (i.e. shipping, which takes place on this part of the channel in high frequency). The high differences between the PECs and the measured environmental concentrations mirror that the water emissions from Rain Carbon contribute only to a minor extent to the overall PAH pollution in the canal.

Table 9-20: Comparison of environmental concentrations found in the canal (~200 m downstream of the emission point) with PEC values for surface water and sediment

	Concentration in surface water [µg/L]					Concentration in sediment [µg/kg dwt] [b]				
	Measurements				PEC	Measurements				PEC
	n [a]	Period	Mean	Maximum	Freshwater	n [a]	Period	Mean	Maximum	Freshwater sediment
Anthracene	7	1991-2013	8.46E-02	2.80E-01	6.31E-05	3	2002-2012	1.67E+03	1.90E+03	1.86E-01
Phenanthrene	6	1991-2013	5.05E-01	1.40E+00	1.06E-04	4	2002-2012	5.08E+03	1.10E+04	2.44E-01
Fluoranthene	7	1991-2013	7.63E-01	1.20E+00	1.15E-04	3	2002-2012	1.51E+04	1.57E+04	1.12E+00
Pyrene	7	1991-2007	7.50E-01	1.40E+00	6.82E-05	3	2002-2012	1.02E+04	1.14E+04	4.02E-01
Benz[a]anthracene	6	1991-2013	1.89E-01	3.60E-01	1.66E-05	5	2005-2012	3.78E+03	7.20E+03	8.33E-01
Chrysene	7	1991-2013	1.86E-01	3.50E-01	2.35E-05	3	2005-2012	7.87E+03	9.00E+03	9.35E-01
Benzo[a]pyrene	5	1991-2007	2.14E-01	4.70E-01	1.27E-05	7	2002-2012	2.71E+03	7.60E+03	1.05E+00
Benzo[k]fluoranthene	7	1991-2013	8.43E-02	2.00E-01	1.09E-05	3	2002-2012	3.30E+03	3.80E+03	8.69E-01
Benzo[ghi]perylene	7	1991-2007	1.35E-01	3.00E-01	7.57E-06	3	2005-2012	5.00E+03	6.10E+03	7.72E-01

[a] n = number of values reported for the given period

[b] No information is provided whether the mean and maximum concentration measured in the canal is given in µg per kg dry weight or wet weight but dry weight is assumed since the concentration is generally indicated as such. The PEC is given in µg per kg dry weight.

Within the scope of a project regarding the renovation and expansion of the plant (details provided in the report: *Project – MER, Hervergunning en uitbreiding PR0429*" [4], in 2008, Rain Carbon Belgium measured the PAH concentrations upstream in the canal, close to their release point (in 160 m distance) and compared them with concentrations measured downstream, at MP 30000 by the Flemish Environmental Agency (VMM) in the same year.

The mean and maximum concentrations calculated for both sites are shown in Table 9-21. All PAH concentrations measured downstream of the release point are lower than upstream. Regarding the mean concentrations, the values measured downstream are by factor 3.5-10 lower while for maximum concentrations they are by factor 3-112 lower than upstream.

These results substantiate that the water emissions from Rain Carbon are negligible compared to the concentrations measurable in the canal. In contrast, the volumes of discharged wastewater apparently dilute the PAH exposure in the canal, due to the relatively low concentration in the emission water.

Table 9-21: PAH concentrations measured in the canal upstream and downstream the point of release (measurements conducted in 2008)

	Mean concentration [µg/L]				Maximum concentration [µg/L]			
	Upstream	Downstr. (MP 30000)	Downstr. - upstream	Reduction factor	Upstream	Downstr. (MP 30000)	Downstr. - upstream	Reduction factor
Anthracene	0.100	0.011	-0.089	9.1	2.230	0.020	-2.210	111.5
Phenanthrene	0.250	0.060	-0.190	4.2	2.020	0.102	-1.918	19.8
Fluoranthene	0.410	0.082	-0.328	5.0	0.590	0.190	-0.400	3.1
Pyrene	0.450	0.074	-0.376	6.1	0.510	0.144	-0.366	3.5
Benz[a]anthra-cene	0.230	0.023	-0.207	10.0	0.460	0.049	-0.411	9.4
Chrysene	0.200	0.027	-0.173	7.4	0.440	0.049	-0.391	9.0
Benzo[a]py-rene	0.090	0.022	-0.068	4.1	0.580	0.050	-0.530	11.6
Benzo[k]fluo-ranthene	0.060	0.009	-0.051	6.7	0.640	0.022	-0.618	29.1
Benzo[ghi]pe-rylene	0.060	0.017	-0.043	3.5	0.500	0.037	-0.463	13.5

[4] *Project – MER, Hervergunning en uitbreiding PR0429;* https://www.milieuinfo.be/dms/d/d/workspace/SpacesStore/4a284860-daf6-417e-b162-45ab1fd94401/TEC0811007SVdB_Rutgers_MER_ev_2.pdf

Air

The air emissions from Rain Carbon originate primarily from off-gas of scrubbers (Table 9-14). Accordingly, for the three PAHs with the highest air emissions (anthracene, phenanthrene and fluoranthene), the highest local and regional concentrations in the atmospheric compartment (local PEC_{air}) were obtained. The local and regional PEC_{air} values are shown in Table 9-22.

Table 9-22: Local and regional PECs for the atmospheric compartment obtained from EUSES modelling

PAH	Annual average local PEC_{air} (total) [ng/m^3]	Regional PEC_{air} (total) [ng/m^3]
Anthracene	9.02E-02	1.18E-06
Phenanthrene	4.89E-01	1.58E-05
Fluoranthene	8.90E-02	2.29E-06
Pyrene	4.41E-02	1.16E-06
Benz[a]anthracene	1.86E-05	1.35E-09
Chrysene	1.86E-05	1.40E-09
Benzo[a]pyrene	1.86E-05	1.30E-09
Benzo[k]fluoranthene	1.86E-05	6.16E-10
Benzo[ghi]perylene	7.01E-04	1.11E-08

Since no PNECs or Environmental Quality Standards are available for the atmospheric compartment, the PEC_{air} values are compared with publicly available data for concentrations of several PAHs measured at survey stations close to the plant. One measurement station, (40ZL01; Havenlaan) is located 150 m east of the plant and a second station (44R750; Burgemeester Jos Chalmetlaan) in Zelzate is positioned in 1.7 km distance, southeast of the plant (in wind direction) in a municipality, where also a steel plant is located (see Figure 9-3). Before 2009, PAHs were measured regularly at both stations, but since 2009, PAH measurements at 40ZL01 were discontinued because the measured concentrations at both stations were comparable. Therefore, PAH measurements from the station in 1.7 km distance are considered representative for PAH emissions close to the plant and are used for comparisons with local PEC_{air} values.

Figure 9-3: Location of the survey stations 40ZL01 and 44R750 in Zelzate

The concentrations of several PAHs measured 2016 at 44R750 (published in the air quality report for the Flamish region "*Luchtkwaliteit in het Vlaamse Gewest Jaarverslag Immissiemeetnetten – 2016*" [5]) are shown in Table 9-23 and compared with the local PEC_{air} values calculated for these PAHs for the emissions from Rain Carbon.

The air concentrations of PAHs measured in different Flamish regions are mostly in the same order of magnitude (XE-01 ng/m^3) and within a range of 0.06 and 0.92 ng/m^3. For the majority of PAHs, the highest concentrations were measured in Sint-Kruis Winkel, most likely influenced by the large steel plant, which is located there. The second highest concentrations of most PAHs (including benzo[a]pyrene) were measured in Zelzate, but influence of traffic (motorways) and also here the steel plant located very close to the survey station (in ~1.5 km distance) may have a distinct impact on the PAH air concentrations. Since the local PEC_{air} values predicted for the emissions coming from Rain Carbon are between one and four (four in case of benzo[a]pyrene) orders of magnitude lower than the concentrations measured at the survey station in Zelzate, emissions from other sources certainly had considerate impacts on these values. Accordingly, with locally measurable PAH background concentrations being much higher than the predicted PEC_{air} values, the environmental effect of Rain Carbon´s PAH emissions to air is negligible.

[5] https://www.vlaanderen.be/nl/publicaties/detail/luchtkwaliteit-in-het-vlaamse-gewest-jaarverslag-immissiemeetnetten-2016

Table 9-23: PAH background concentrations in air (2016), compared with calculated local PEC_{air} values (all values in ng/m³)

	Borgerhout-straatkant	Genk	Ghent	Grimbergen	Grimbergen (12m)	Houtem	Kallo	Sint-Kruis-Winkel	Zelzate [a]	Average (all regions) [b]	PEC_{air} local
Flouranthene	2.50E-01	1.40E-01	1.80E-01	1.20E-01	1.50E-01	8.00E-02	1.20E-01	3.00E-01	2.10E-01	1.80E-01	8.90E-02
Pyrene	2.30E-01	1.40E-01	1.70E-01	1.30E-01	1.70E-01	8.00E-02	1.10E-01	2.50E-01	1.90E-01	1.70E-01	4.41E-02
Benz[a]anthracene	1.40E-01	1.00E-01	1.40E-01	1.00E-01	1.30E-01	6.00E-02	7.00E-02	2.40E-01	1.70E-01	1.30E-01	1.86E-05
Chrysene	3.30E-01	2.50E-01	3.30E-01	2.20E-01	2.90E-01	1.50E-01	2.00E-01	4.60E-01	3.50E-01	3.00E-01	1.86E-05
Benzo[a]pyrene	1.70E-01	1.50E-01	1.80E-01	1.50E-01	1.90E-01	8.00E-02	1.00E-01	2.60E-01	2.00E-01	1.70E-01	1.86E-05
Benzo[b+j+k]fluo-ranthene	5.20E-01	5.10E-01	5.80E-01	4.50E-01	5.60E-01	3.20E-01	3.90E-01	9.20E-01	6.70E-01	5.60E-01	3.72E-05 [b]
Benzo[ghi]pery-lene	2.30E-01	2.10E-01	2.50E-01	2.10E-01	2.50E-01	1.30E-01	1.60E-01	3.30E-01	2.50E-01	2.30E-01	7.01E-04

[a] Station 44R750, located 1.7 km southeast of Rain Carbon (in wind direction).

[b] The sum of PEC_{air} values only for benzo[b]fluoranthene and benzo[k]fluoranthene is provided since benzo[j]fluoranthene is not subject to this AfA and was not measured. Note that benzo[b]fluoranthene is not PBT and the environmental modelling was only performed as the substance is required for calculating the sum of 4 EFSA PAHs for the assessment of HvE.

This conclusion can be substantiated by comparing the regional PEC_{air} values (Table 9-22) with PAH concentrations measured in Flamish regions (Table 9-23) and with publicly available background concentrations of benzo[a]pyrene measured at stations throughout Belgium (Table 9-24).

The mean and maximum background concentrations of benzo[a]pyrene in urban and suburban Belgian environments (Table 9-24) are in the same order of magnitude as the concentrations measured in Zelzate in 2016 (0.2 ng/m^3; Table 9-23). This applies for both, measurements where it was not defined if benzo[a]pyrene was particle-bound or not, and measurements of benzo[a]pyrene in particulate matter with an aerodynamic diameter smaller than 10 µm (PM_{10}).

The local PEC_{air} value for benzo[a]pyrene (Table 9-22; 1.86E-05 ng/m^3) calculated for emissions from Rain Carbon is between three and four and the regional PEC_{air} value (Table 9-22; 1.30E-09 ng/m^3) is between six and eight orders of magnitude lower than these environmental concentrations. This supports the assumption that the PAH air emissions from Rain Carbon are negligible compared to the PAH concentrations measured in the local and regional environment.

Table 9-24: Measured air concentration of benzo[a]pyrene in Belgium, 2015

Station area	BaP (not defined if particle-bound or not) [ng/m^3]			BaP in PM_{10} [ng/m^3]		
	Mean	Min	Max	Mean	Min	Max
rural	-	-	-	9.42E-02	5.06E-02	1.38E-01
suburban	1.20E-01	8.31E-02	1.44E-01	1.80E-01	7.26E-02	2.76E-01
urban	1.85E-01	1.85E-01	1.85E-01	1.45E-01	1.32E-01	1.58E-01
all	1.53E-01	8.31E-02	1.85E-01	1.40E-01	5.06E-02	2.76E-01
Sub-urban + urban	1.53E-01	8.31E-02	1.85E-01	1.62E-01	7.26E-02	2.76E-01

Source: European Environment Agency [6]; file: ***Air pollutant concentrations 2015 (compared to EU values)***

Summary – Exposure for the environment

The environmental concentrations calculated by EUSES modelling are much lower than the PNECs or background concentrations which can be found for the compartments freshwater and freshwater sediment, soil or air. Accordingly, the environmental impact coming from the water and air emissions from formulation activities with CTPht and AO at Rain Carbon is negligible. Moreover, the calculated values overestimate the real exposure conditions due to the following reasons:

[6] https://www.eea.europa.eu/data-and-maps/data/air-pollutant-concentrations-at-station; accessed on 23th November 2018;

- The only water emission source relevant for formulation activities at Rain Carbon is water coming from WWTP 2. However, not only the rainwater from the entire concrete surface of the plant is led to WWTP 2, it also receives the effluents from WWTP 1, which is dedicated to the process surface of the tar refinery, incl. the cleaning box. Also other waters used for technical applications and water from steam production and use are led to on-site WWTP 2. Since only the rainwater and to a small extent water arising in the cleaning box from the cleaning of parts is relevant to formulation activities, the emissions coming from all other sources, which are included in the emission data used for EUSES calculations (Table 9-15), overestimate the real exposures from formulation activities. As a rough estimate, 25-30% of these emissions come from sources other than the rainwater.
- Even considering only the rainwater fraction in the whole effluent of WWTP 2 as relevant water emission this is still an overestimation, since the rainwater from the surface of the whole plant (35 200 m^2) is led to WWTP 2, but only 34% of the surface area are assigned to the formulation activities (surface total plant: 35 200 m^2; surface area of the pitch tank farm and the pitch blending area: 9 000 m^2, 9 000 m^2/35 200 m^2 = 25.6%; surface area of the tank farm for oil blending: 3 000 m^2, 3 000 m^2/35 200 m^2 = 8.5%; sum of the two relevant surface areas = 34.1%). Accordingly, the (already negligible) calculated local PECs for the water and sediment compartment effectively overestimate the real exposures from formulation activities by the factor of 3.
- Furthermore, the local PECs for the freshwater and sediment compartment may be considered overestimated by an additional factor of 3.7, since a dilution factor of 1 000 was applied for the water emissions into the canal, although the actual dilution factor would be 3 712 (as described above for the EUSES input parameters; the usage of a dilution factor >1 000 would not be in accordance with the Guidance on Information Requirements and Chemical Safety Assessment Chapter R.16: Environmental exposure assessment, version 3.0 (ECHA, 2016).
- The air emission values used for EUSES calculations (Table 9-14) also lead to an overestimation of the real exposure concentrations since only 66% of the emissions coming from scrubber K100A (connected to the storage park for tar oils) are relevant for formulation activities.

Relative contributions of CTPht and AO to PAH emissions to the environment

From the overall emissions (to surface water and air) coming from formulation activities with CTPht or AO (as provided in Table 9-16), AO contributes most of the amount of anthracene and phenanthrene, one half of fluoranthene and one third of pyrene, as shown in Table 9-25. The other PAHs are not contained in AO in relevant amounts.

Table 9-25: Tonnages and relative amounts of CTPht, AO and the individual PAHs used in formulations relevant for this AfA

	Content CTPht		Content AO		% CTPht	% AO
	[%] [a]	[tpa] [c]	[%] [b]	[tpa] [c]		
Tonnage CTPht		[redacted]		* [d]		
Tonnage AO				[redacted]		
Anthracene	0.057	[redacted]	6.11	[redacted]	6.8	93.2
Phenanthrene	0.302	[redacted]	25.92	[redacted]	8.3	91.7
Fluoranthene	0.835	[redacted]	6.37	[redacted]	50.6	49.4
Pyrene	0.726	[redacted]	2.85	[redacted]	66.6	33.4
Benz[a]anthracene	0.599	[redacted]			100.0	0.0
Chrysene	0.835	[redacted]			100.0	0.0
Benzo[a]pyrene	0.873	[redacted]			100.0	0.0
Benzo[k]fluoranthene	0.393	[redacted]			100.0	0.0
Benzo[ghi]perylene	0.550	[redacted]			100.0	0.0

Unrounded values were used for calculations.

[a] According to the European Composite Sample for CTPht

[b] According to the European Composite Sample for AO

[c] tpa = tonnes per annum

[d] Total AO ~ [redacted]; tonnage of EU Creosote not considered ([redacted] tpa); relevant tonnage = [redacted] tpa.

9.1.2.4 Exposure and risks for humans via the environment from CTPht

The handling of CTPht may lead to exposure of humans to PAHs via the environment. The local and regional PEC_{oral} and PEC_{air} values were obtained from EUSES modelling. Due to the very conservative nature of the EUSES modelling of the intake via food more adequate food consumption data were used (as described above in the approach to EUSES modelling).

The results were used to calculate the excess lifetime cancer risks (ELCRs) for different types of cancer. The ELCRs were calculated by multiplying the exposures (local/regional PEC_{oral}/PEC_{air}) with the exposure-risk relationships as given in section 9.0.3. The PECs and the obtained ELCRs are shown in Table 9-26 on a local and in Table 9-27 on a regional scale.

Table 9-26: Local PEC_{oral} and PEC_{air} (obtained from EUSES modelling), used for calculation of excess life cancer risks (ELCRs)

Exposure route	Explanation	Benzo[a]-pyrene	Chrysene	Benzo[b]-fluoranthene	Benz[a]-anthracene	Sum PAH4 EFSA	Risk estimate for cancer per ng PAH4/kg bw/day	Risk estimate for cancer per 1 ng BaP/m^3 (excess lifetime cancer risk)		ELCR
Oral general population	Total daily intake oral (PEC_{oral}) for individual PAHs [ng/kg/d]	3.03E-03	4.99E-02	2.83E-01	2.37E-03					
	Total daily intake oral (PEC_{oral}) for sum PAH4 EFSA [ng/kg/d]					3.38E-01	2.06E-06			**6.97E-07**
Inhalation general population	Annual average local PEC in air (total) [ng/m^3]	1.86E-05						lung	3.00E-05	**5.58E-10**
								bladder	2.10E-05	**3.91E-10**
								total (lung & bladder)		**9.49E-10**
Workers onsite (not involved in formulation activities)	Annual average local PEC in air (total) [ng/m^3]	1.86E-05						lung	5.60E-06	**1.04E-10**
								bladder	4.00E-06	**7.44E-11**
								total (lung & bladder)		**1.79E-10**

Table 9-27: Regional PEC_{oral} and PEC_{air} (obtained from EUSES modelling), used for calculation of excess life cancer risks (ELCRs)

Exposure route	Explanation	Benzo[a]-pyrene	Chrysene	Benzo[b]-fluoranthene	Benz[a]-anthracene	Sum PAH4 EFSA	Risk estimate for cancer per ng PAH4/kg bw/day	Risk estimate for cancer per 1 ng BaP/m^3 (excess lifetime cancer risk)		ELCR
Oral general population	Total daily intake oral (PEC_{oral}) for individual PAHs [ng/kg/d]	3.66E-06	7.30E-05	3.11E-04	2.48E-06					
	Total daily intake oral (PEC_{oral}) for sum PAH4 EFSA [ng/kg/d]					3.90E-04	2.06E-06			**8.04E-10**
Inhalation general population	Regional PEC in air (total) [ng/m^3]	1.30E-09						lung	3.00E-05	**3.90E-14**
								bladder	2.10E-05	**2.73E-14**
								total (lung & bladder)		**6.63E-14**

As can be seen from the tables above, for both the local and regional scale the oral exposure dominates the exposure of humans via the environment. Drinking water contributes to less than 7% to the overall oral exposure, which is locally (Table 9-28) and regionally (Table 9-29) dominated by uptake of PAHs via fish. This high fraction of PAHs in fish comes from the high BCF values of the PAHs, which are expected to accumulate in fish.

Table 9-28: Fractions of daily human dose: local assessment

Fraction of daily dose through diverse intake pathways								
	Drinking water	**Fish**	**Leaf crops**	**Root crops**	**Meat**	**Milk**	**Air**	**Sum of all fractions**
Benz[a]anthracene	0.0500	0.6240	0.2000	0.0012	0.0883	0.0348	0.0022	1.00
Chrysene	0.0034	0.9820	0.0094	0.0001	0.0034	0.0013	0.0000	1.00
Benzo[a]pyrene	0.0298	0.8690	0.0467	0.0016	0.0369	0.0145	0.0018	1.00
Benzo[b]fluoranthene	0.0006	0.9970	0.0014	0.0000	0.0011	0.0004	0.0000	1.00

Unrounded values used for calculation.

Table 9-29: Fractions of daily human dose: regional assessment

Fraction of daily dose through diverse intake pathways								
	Drinking water	**Fish**	**Leaf crops**	**Root crops**	**Meat**	**Milk**	**Air**	**Sum of all fractions**
Benz[a]anthracene	0.0643	0.8030	0.0140	0.0987	0.0144	0.0057	0.0002	1.00
Chrysene	0.0034	0.9910	0.0005	0.0046	0.0005	0.0002	0.0000	1.00
Benzo[a]pyrene	0.0287	0.8370	0.0028	0.1140	0.0122	0.0048	0.0001	1.00
Benzo[b]fluoranthene	0.0006	0.9910	0.0009	0.0064	0.0010	0.0004	0.0000	1.00

Unrounded values used for calculation.

Although representative food consumption data of the Belgian population were used instead of the very conservative EUSES default values, the oral intake calculations remain conservative (the consersvatism of the EUSES food modelling is also acknowledged in the Guidance on Information Requirements and Chemical Safety Assessment Chapter R.16: Environmental exposure assessment (version 3.0; ECHA, 2016)).

Two factors contribute to the relatively high modelled oral exposure for the local and regional scenario:

- The oral exposure calculation by EUSES assumes that all food items consumed (root crops, leaf crops, milk, meat and fish) by the local population are sourced from the vicinity of the site, which is unrealistic. Note that under “leaf crops” EUSES actually summarises the following food groups:
    - vegetables

- fruits and nuts
- cereals and cereal products

and for all of them it is assumed that they come 100% from the immediate surroundings of the source (1 000 m radius).

- The same holds true for "fish". Note that the model assumes that all fish consumed is caught in the canal, which is an unrealistic assumption. Actually, since all water emissions from formulation activities at Rain Carbon are discharged into the canal and from there led to the sea, it can reasonably be assumed that a low portion of the emitted substances comes into contact with areas where food is produced.

Further, as described above, the calculated exposure levels and ELCRs effectively overestimate the real exposures and risks coming from discharged water related to formulation activities by the factor of 3. With considering the total water volume from the on-site WWTP 2 as rainwater, the rainwater from the surface of the whole plant was regarded as emission source for EUSES modelling, but only 34% of the surface are assigned to the formulation activities.

We consider this by reducing the risks calculated with EUSES for oral exposure in the local assessment

- by the factor of 5 to account for the fact that EUSES assumes 100% origin from the surroundings of the source (local assessment, assuming 20% consumption of homegrown products and self-caught fish from the canal)
- by the factor of 3 for taking into account that only 1/3 of the emissions can be attributed to formulation activities.

Considering also that a dilution factor of 1 000 was applied for the water emissions into the canal although the actual dilution factor would be 3 712, the exposures and risks coming from water discharges are overestimated by an additional factor of 3.7. This adds to the conservativism of the approach.

The following tables provide the final risk calculation for the local (Table 9-30) and regional (Table 9-31) scenario.

Table 9-30: Calculation of excess life cancer risks (ELCRs): local assessment

Exposure route	Source / justification	ELCR
Oral **general population**	value calculated in Table 9-26 above, divided by factor 15:	**4.65E-08**
Inhalation **general population**	as calculated in Table 9-26 above: total (lung & bladder)	**9.49E-10**
Workers onsite (not involved in formulation activities)	as calculated in Table 9-26 above: total (lung & bladder)	**1.79E-10**

Table 9-31: Calculation of excess life cancer risks (ELCRs): regional assessment

Exposure route	Source / justification	ELCR
Oral **general population**	value calculated in Table 9-27 above:	**8.04E-10**
Inhalation **general population**	as calculated in Table 9-27 above: total (lung & bladder)	**6.63E-14**

Considerations on uncertainty regarding air emission data:

As explained in chapter 9.1.2.2 release data from 2009 were preferred over those from 2018, because releases of PAHs considered PBT substances were higher in 2009 (by a factor of approximately 2). Release rates to air for the four EFSA PAH were higher in 2018 by approximately a factor of 10, although the release rate of benzo[a]pyrene was only higher by factor 2 in 2018. We performed a sensitivity analysis for the assessment of humans via the environment to be able to judge on the consequences. In Annex XII the 2018 emission data are shown as used for a comparative calculation of exposure of HvE as given in Annex XIII:

These calculations show that even with the emission data from 2018, where the total air emission of the 4 EFSA PAHs relevant for the assessment of HvE was higher than in 2009 by a factor of 10, the local and regional PEC_{oral} and PEC_{air} values for these 4 PAHs (Tables in Annex XIII) are only slightly higher than the ones obtained for the emission data from 2009. If the assessment would have been based on the air emission data from 2018, the resulting excess life cancer risks (ELCRs) for the local and regional population would be nearly identical for oral exposure (local: factor 1.10, regional: factor 1.01 higher) and higher by factor of approximately 2 (local: factor 2.17; regional: factor 1.38) for exposure via inhalation (see PEC_{oral}, PEC_{air} and ELCR values for the local and regional assessment provided in Annex XIII). This is due to two factors:

- the higher emissions to air do not have a large impact on the oral exposure, and, hence, on the overall risk (as oral exposure is dominating the overall risk)
- the inhalative risk is calculated based on the benzo[a]pyrene concentration, which is only two times higher based on 2018 data (as emission for that substance is also only two times higher in 2018).

The sensitivity analysis shows that using the 2018 data results in the same risk for humans via the environment, whereas for the environmental assessment of PBT substances use of 2009 data remains the more conservative approach.

<u>Summary – Exposure and risks for man via the environment</u>

The ELCRs indicate that the cancer risks for humans exposed via the environment to the formulation activities **with CTPht** (formulation activities with AO are not assessed for human health risks) are low due to the low exposure levels coming from the plant of Rain Carbon. Despite the conservative modelling, calculated risks from exposure of humans via the environment are well below the 10^{-6} level (local and regional) for the whole emissions of the plant from rainwater to water and from emissions to air.

9.1.3 Worker contributing scenario 1 – PROC 3 and PROC 8b – Plant and logistics operators

9.1.3.1 Conditions of use

Table 9-32: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture: 50-99% CTPht in pitch mixtures • Physical form of the used product: liquid
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: ≤8 h/day
Technical and organisational conditions and measures
• Closed process with occasional controlled exposure • Exhaust air recovery systems for tanks and loading stations, incineration of exhaust air
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes, during specific tasks with potential dermal exposure such as sampling • Respiratory Protection: Yes, during specific tasks with potential exposure via inhalation such as sampling • Eye protection: Yes, during specific tasks with potential exposure to eyes such as sampling • Working clothes: Yes • Protection boots: Yes • Helmets: Yes
Other conditions affecting workers exposure
• Place of use: Outdoor • Operating temperature: ≤30 °C (in tasks related to potential exposure such as sampling)

9.1.3.2 Exposure and risks for workers

The group of operators involved in the formulation processes consists of 22 (21 + 1) people working at the tar plant. Every shift is composed of three workers:

- Chief operator
- Plant operator
- Logistics operator

One operator, the 22nd person, works on small batch formulations (in day service only; AO formulations, does not include CTPht).

Plant operators

Operators are mainly responsible for surveying and steering the tar distillation and refinery installations (not related to formulation; their tasks in managing the tar refinery are: manipulating manual valves, reading of manual gauges, sampling of the different cuts for quality control, surveillance walks, surveys of the technical equipment, supervision, communication with other operators). During most of their labour time, the operators supervise these processes and control the production parameters. They are not routinely present at the tank farm and come as support of the logistics operators on demand. Therefore, their time spent on activities related to the formulation process of pitch mixtures constitutes only a small portion of their overall work, a conservative estimate being not more than **10%.**

When performing tasks at the tank farm involving formulation activities, their main tasks are surveying the automated mixing process (consisting of walks at the tank farm and of time spent in the control room) and taking samples (see below).

Chief operators

Chief operators are responsible for surveying all activities. They operate mainly from the control room and are rarely engaged in plant walks or other activities outside. The actual contribution of formulation activities to their overall activities are difficult to assess, but are certainly even lower than those for plant operators. Conservatively, 10% (same as for plant operators) are assumed for chief operators.

Logistics operators

Logistics operators are responsible to run the tank farm, where formulation is done. Their tasks include un-/loading of ships and tank trucks (e.g. manoeuvring the loading neck into and out of the manhole during loading), taking samples of the mixtures and transporting them to the laboratory, manipulating manual valves, reading of manual gauges. All storage / logistics of substances at Rain Carbon is liquid. The plant has no possibilities to handle solid products (e.g. solid pitch).

The formulation procedure consists essentially of pumping products around in closed tanks / piping systems. Apart from un-/loading activities, the main activities where logistics operators are involved in formulation activities are sampling, opening/closing of valves and starting/stopping pumps. Although the formulation in the equipment may take several days, the effective operation time might be only 10 min: set the valve and start the pump. Occasionally, they provide assistance for maintenance workers, preparing the system for intervention in case a maintenance case occurs, cleaning of technical equipment.

<u>Sampling</u>

Approximately 455 samples of pitch mixtures are taken from the tank farm (where formulation takes place) per year. Most of the time attributed to sampling involves no exposure risk: getting a sample container, logging the sample in the Laboratory Information Management System (LIMS), printing and applying the label, going to the sampling point,

transporting the sample to the laboratory. The actual sampling moment with hot product close / manipulation of the solidified sample takes approximately 5 min per pitch mixture sample.

Pitch sampling points allow conducting the entire sampling procedure in a closed system under very controlled conditions. The operator takes samples from outlets installed at the pipes which are enclosed by sampling boxes (with glass doors; see photos which are provided in Annex X). All of the sampling boxes are connected to a ventilation system for fume off-take and are connected to activated carbon air treatment.

The operator opens the glass door, places an aluminium dish (341 x 223 x 24 mm, approx. 1 300 mL capacity) into the sampling box, closes the glass door and presses a button in order to start a fan/ pump which creates draft/local exhaust ventilation in the box. Then he opens the pipe via a little wheel at the manual valve for ca. 20 seconds (controlled flow-rate). The pitch mixture is sampled into the open aluminium dish within the closed sampling box. The dish remains into the sampling box until the sample is completely solidified (2-3 min). Meanwhile, the vapour emerging from the sample is extracted from the box via an off-gas pipe which is connected to the fan. The drawn-off air is lead into an active carbon filter in a barrel next to the sampling box. When the pitch mixture sample is solidified, it is taken out of the sampling box, put into a plastic bag and transported to the lab, where it is placed from the outside through a hatch into a fume hood. The duration for the complete sampling procedure including the delivery is approximately 5 min for sampling + 5 min for transport of the solidified sample in the closed bag per sample.

Ship loading

All CBF and AO mixtures for export, as well as most (approximately 90%) of the pitch mixtures produced at Rain Carbon are delivered to the customers via vessels (typical vessel batch size 150-12 000 t, 66% >1 000 t, average 1 800 t). Between [redacted] (0-300) ship loadings with around [redacted] (0-300 000) t CTPht contained in pitch mixtures are conducted in total per year.

After the formulation process is completed, the mixture is pumped via closed lines from the mixing tank to a dedicated ship loading station. In case of pitch mixtures, the ship loading is conducted at elevated temperature in order to avoid pitch solidification within the closed lines. Two workers are involved in the preparations of ship loading, one worker from the mechanical workshop and one loading operator. The worker from the mechanical workshop connects the flange connections of the hoses onto the manifold of the ship. A wireless pressure transducer is mounted between the ship's manifold and shore vapour return line. This enables the control room to see pressure on the ship. The total procedure time is approximately 30 min, during which the loading operator handles the two hoses for approximately 15 min. Once the hoses are connected, the workers leave the ship loading station. The ship is monitored by camera and a supervisor, who is in communication with the control room via a radio connection, is positioned on deck. The pumps are started from the control room and the ships are loaded with the mixture. Depending on the delivery volume on the vessel and the flow rate (200 t per h for small ships, 400 t per h for big ships), the whole loading procedure takes between 5 and 25 h. After the loading is completed, the

pumps are turned off and the lines are closed. The remains within the hoses are drained and blown out with air onto the ship. The hoses are closed with a blind flange for storage.

Tank truck loading

Small quantities of pitch mixtures are delivered via tank trucks (25 t per truck) to the customers. Per year, approximately [redacted] (0-1 500) tank trucks are loaded with pitch mixtures, accounting for approximately [redacted] (0-40 000) t of pitch mixtures per year in total.

The whole tank truck loading procedure is conducted in a closed system. After the formulation process is completed, the pitch mixtures are pumped via closed lines from the storage tank to a dedicated filling station for tank trucks. The truck loading occurs at elevated temperature (220-230 °C). Truck transportation has a limited range, as pitch trucks are not able to heat the product.

When the truck enters the truck loading station for pitch mixtures, the truck driver, an external service provider, opens the manhole and then retreats back into the drivers cabin. A scale is included in the floor of the loading station is a scale, so the filling degree of the truck can be monitored/controlled with this external device. The logistics operator enters the loading station and manoeuvres the loading cone (equipped with two lines; one with the product, one for exhaust air recovery to prevent emissions) with pneumatic power into the manhole (3 min). The cone pneumatics push the cone down on the manhole. Afterwards the logistics operator is obliged to leave the loading station to a shelter close to where the weight indication of the scale can be monitored. The logistics operator then calls the chief operator in the control room via the radio to start the loading operation. The duration of the whole loading procedure is approximately 30 min for one tank truck. After the tank is filled, the operator removes the loading cone pneumatically from the manhole, closes the cover of the manhole on the truck and places a stainless steel bucket below the pitch line to catch the drops that might fall. These drops solidify fast and are collected and discharged as waste. The logistics operator then moves the arm back to its resting position (3 min.). The truck driver locks the manhole and drives the truck off. No samples are taken during truck loading.

During performance of their tasks, operators wear specific PPE:

- Working clothes
- Helmet
- Gloves:
    - Heavy duty SHOWA 720R nitrile gloves (thickness 1.1 mm) are worn as standard operator gloves for occasional contact,
    - A long sleeve version of the nitrile heavy duty glove (thickness 0.5 mm) is equally available
    - For high temperature works neoprene gloves (thickness 1.6 mm) with cotton jersey liner are used (Ansell Scorpio 09-022)
    - In case of anticipated more intense product contact Viton gloves (thickness 0.3 mm) are available.
- Full mask (in case they have to perform an operation that could lead to pitch vapours exposure), filter ABEK P3

The following table provides an overview on the working times spent by logistics operators on different types of activities/products. Note that these times also include respective sampling activities.

Table 9-33: Tar refinery logistics operator job content on a yearly basis

	Procedures in 2017	Duration [h]	Total [h]	Running total [h]	[%]
CTPht ships	[redacted]	0.75	[redacted]	81	**5**
CTPht trucks	[redacted]	0.5	[redacted]	608.5	**33**
AO mixtures ships	[redacted]	0.75	[redacted]	660.25	3
EU creosote trucks*	[redacted]	0.5	[redacted]	1 060.25	25
Formulation of CTPht		1h/day	273	1 333.25	**17**
Formulation of AO		1h/day	273	1 606.25	17

* EU creosote: estimate for 2018 onwards

It can be concluded that in total logistics operators spend maximum 55% (contributions from activities in bold in table above) of their time on CTPht and its formulation.

Description of data used for assessment of workers' exposure

Regular biomonitoring campaigns are conducted at Rain Carbon. In the following (Table 9-34), data obtained from campaigns through the years 2012-2018 are reported.

Table 9-34: Number* of individual workers monitoring 2012 – 2018 (SD: shut-down periods, NO: normal operation)

Job		2012	2013	2014	2015	2016	2017	2018	Total
Operators	smokers SD	-	3	-	3	-	2	-	8
	non-smokers SD	-	2	-	1	-	2	-	5
	smokers NO	-	3	7	3	2	2	-	17
	non-smokers NO	**4**	**1**	**3**	**2**	**9**	**1**	**-**	**20**
Chief operators	smokers SD	-	1	-	-	-	-	-	1
	non-smokers SD	-	2	-	4	-	3	-	9
	smokers NO	-	1	1	1	-	-	-	3
	non-smokers NO	**1**	**1**	**2**	**3**	**8**	**4**	**-**	**19**
Logistics operators	smokers SD	-	-	-	-	-	-	-	0

	non-smokers SD	-	-	4	4	3	3	6	20
	smokers NO	-	-	-	-	-	-	-	0
	non-smokers NO	**4**	**3**	**5**	**6**	**10**	**3**	**2**	**33**
total		11	17	22	27	32	20	8	135

*Only individuals with all 4 samples (i.e. day 1 and 5 pre- and post-shift) available were counted

During these campaigns pre- and post-shift measurements on day 1 and day 5 of the work week were taken. A description of methods is provided in Annex XI and summary statistics are provided as a separate (confidential) document. Workers are split according their job description and smoking status (non-smokers and smokers).

For those with higher exposures (both smokers and non-smokers) levels increased from pre- to post-shift and from day 1 to day 5. Although the database depicts some variability, smokers had consistently higher levels (by approx. factor 1.5 to 3), clearly indicate a relevant contribution of smoking to the total burden of PAHs.

Approximately 31% of values for the various types of operators were measured during performance of the general shutdown of the tar refinery (as these activities can potentially lead to higher exposures they are in the focus of occupational safety surveillance activities of the company). As explained above, general shutdowns do not relate to formulation activities, as these are not subject to annual maintenance activities. Therefore, these values are excluded from further consideration. The remaining measurements were taken during normal production routines and include all typical activities as described above for the different types of operator jobs.

In the following, the exposure assessment is based on all measurements from 2012 to 2018 for non-smokers (normal operation, see in bold in Table 9-34) for

- all three types of operators (separately)
- non-smokers (to exclude the contribution to PAH exposure from smoking)
- end-of-shift on day 5.

In a conservative way the risk characterisation is based on 90th percentiles, although for calculating cancer risks the long-term average exposure is more relevant.

Table 9-35: Results from biomonitoring campaigns 2012 – 2018; all values are given as 1-hydroxypyrene in urine [µg 1-OHP/g creatinine], measured on day 5, end of shift; 90th percentile values used for risk characterisation (normal production, non-smokers only)

Job description	n	AM	STD	90th percentile
Operators	20	1.89	0.98	2.96
Chief operators	19	0.93	0.76	1.76
Logistics operators	33	2.31	1.38	3.94

The measured values are given with the unit µg 1-hydroxypyrene/g creatinine. These values are converted with the divisor 1.93 (molecular weight of 1-OHP of 218.26 g/mol, divided by

molecular weight of creatinine of 113.12 g/mol) into values with the unit µmol/mol creatinine.

For converting this to a BaP workplace air concentration the equation as given in ECHA (according to 2018) is used:

BaP workplace air concentration [ng/m^3] = ((1-OHP urinary concentration [µmol/mol creatinine] – 1.13)/11.1) x 1 000

In Table 9-36, 90th percentile values for the three different groups of workers as shown in Table 9-34 are converted into BaP air concentrations.

Table 9-36: Transformation of 1-hydroxypyrene levels (90th percentiles) into BaP workplace air concentrations

Job description	1-OHP in urine [µg/g creatinine]	1-OHP in urine [µmol/mol creatinine]	Corresponding conc. of BaP in workplace air [ng/m^3]
Operators	2.96	1.53	36.4
Chief operators	1.76	0.91	-
Logistics operators	3.94	2.04	82.2

Excess lifetime cancer risks per job description are calculated for operators (Table 9-37) and logistics operators (Table 9-38) based on these 90th percentile values, taking into consideration the share of time spent on formulation activities and using the exposure-risk relationship as published by RAC (ECHA, 2018).

Table 9-37: Excess lifetime cancer risks (ELCRs) for operators (n = 7 workers)

Target organ:	Long-term exposure [ng BaP/m^3] *	% of time related to formulation	Corrected concentration [ng BaP/m^3]	Risk estimate for cancer per ng BaP/m^3 (40 years of occupational exposure)	ELCR
	36.4	10%	3.64		
Lung				5.60E-06	2.04E-5
Bladder				4.00E-06	1.46E-5
Combined					3.50E-5

* Based on 90th percentile biomonitoring values

Table 9-38: Excess lifetime cancer risks (ELCRs) for logistics operators (n = 7 workers)

Target organ:	Long-term exposure [ng BaP/m^3] *	% of time related to formulation	Corrected concentration [ng BaP/m^3]	Risk estimate for cancer per ng BaP/m^3 (40 years of occupational exposure)	ELCR
	82.2	55%	45.21		
Lung				5.60E-06	2.53E-4
Bladder				4.00E-06	1.81E-4

Combined					4.34E-4

* Based on 90th percentile biomonitoring values

No excess lifetime cancer risks are calculated for chief operators. As expected their exposure levels are lower than those of the other operators. As their 1-OHP levels are below 1.13 µmol/mol creatinine (90th percentile 0.91 µmol/mol creatinine), it can be reasonably assumed that their exposure is not far from background exposure levels. Furthermore, only a small part of their activities is actually dedicated to formulation processes.

Discussion

The data in Table 9-35 show that on average workers in these groups have 1-OHP values below 2.31 µg/g creatinine or 1.2 µmol/mol creatinine for logistics operators and values below 1.89 µg/g creatinine or 0.98 µmol/mol creatinine for plant operators. According to RACs exposure-risk relationship this relates to a very low exposure to PAH via air and a very low to negligible cancer risk (1-OHP levels below 1.13 µmol/mol creatinine are not associated with an increased cancer risk due to workplace exposure).

The higher 90th percentile values show that occasionally higher exposures might occur. By using the 90th percentile values for the risk characterisation means that it is assumed that

- individual workers are exposed daily for 40 years at this level
- all workers in the group are exposed at that high level.

With these very conservative assumptions the calculated risks are in the range of 3.5 x 10^{-5} for plant operators and 4.34 x 10^{-4} for logistics operators, taking into account the actual time spent on formulation activities. Chief operators seem to have no significantly increased PAH exposure compared to background levels.

Dermal exposure

The use of the biomonitoring data and the transformation into BaP air concentrations was done under the assumption that dermal exposure contributes to a negligible extent to total exposure. This assumption is based on the use conditions:

- all materials containing CTPht are used at high temperatures only, which would immediately cause severe burns
- the company's medical history documents that such incidents are extremely rare (2 cases for the whole plant (not necessarily formulation processes) in the last 10 years)
- workers are using adequate personal protection equipment to minimise any potential for skin contact
- any outside contamination of objects is immediately detected due to the black colour of all mixtures containing CTPht.

Conclusion on risk characterisation:

Calculated extra cancer risks are

- 3.50 x 10^{-5} for 7 plant operators
- 4.34 x 10^{-4} for 7 logistics operators.

9.1.4 Worker contributing scenario 2 – PROC 15 – Laboratory technicians

9.1.4.1 Conditions of use

Table 9-39: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture: 50-99% CTPht in pitch mixtures • Physical form of the used product: liquid
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: ≤8 h/day
Technical and organisational conditions and measures
• Fume cupboards : the flow with open door is >40 cm/sec, flow control system installed • Variable Air Flow System in the laboratory; number of renewals (air change/h): 10-12
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes, during specific tasks with potential dermal exposure such as sample handling • Respiratory Protection: No • Eye protection: Yes, during specific tasks with potential exposure to eyes such as sample handling • Working clothes: Laboratory coat • Protection boots: No • Helmets: No
Other conditions affecting workers exposure
• Place of use: Indoor • Operating temperature: 30-120°C

9.1.4.2 Exposure and risks for workers

The typical working time of a laboratory technician is 1 530 h/year (2017), accounting for 7 650 working h/year in total for the five laboratory technicians working in shift (who process most of the pitch samples).

Numbers of pitch mixture samples:

- From tank farm (formulation): ±455 samples/year (accounting for ±2.1% of the production samples handled by the laboratory technicians). Typical handling time is 80 min/sample (80 min x 455 = 606.7 h).
- For shipments (incoming and outgoing ships): ±140 samples/ year (accounting for ±7% of all shipments samples handled by the laboratory technicians). Typical handling time is 120 min/sample (120 min x 140 = 280 h).

The samples are handled by the laboratory technicians after the operator transported the aluminium dishes (for pitch mixture samples) to the laboratory and placed them (from outside the building) through a hatch into the sample reception cupboard/ fume hood.

The fume hood with the hatch is the starting point for all samples. From there, samples are taken out and subjected to the different analyses steps. Solidified pitch samples are milled and crushed (particle size 200-300 µm) before they are analysed, in a hood with particle filter on the exhaust to atmosphere outside the lab. In case liquid samples are required for individual tests, small portions of solid material are liquefied by heating under the hood.

Each test is performed within a separate fume hood, dedicated to the respective analysis. Every fume hood is equipped with a standard operating procedure for the respective type of analysis. The functionality and air exchange volumes of the fume hoods are constantly monitored by an under-pressure monitoring unit with automated alert function which gives visual and audible warnings in cases of insufficient air flow. The laboratory is equipped with four GC-MS devices (1 g of the sample is needed for GC-MS), one for water analysis, two for product analysis (e.g. analysis of benzo[a]pyrene content as continuous routine; max 50 ppm in AO) and one for experimental tests on different matrices.

The principal tests conducted by laboratory technicians on pitch mixtures are:

- Softening point (with liquefied sample, approximately 30 mL) ASTM D3104
- Trace metals determination (via X-ray Fluorescence)
- Determination of viscosity ASTM D5018
- Determination of solubility in solvents DIN 51906/ DIN 51921
- Determination of coking residue DIN 51905
- Determination of ash residue ISO 8006
- Determination of carbon content ASTM D5291 mod

At the end of all analyses steps, the solid samples are discarded into a waste bin located in the first fume hood with the hatch. The waste bin is taken out of the hood through the hatch and emptied approximately two times per shift into the closed container for solid waste which is located on the plant, close to the laboratory. The samples are discarded as hazardous waste and incinerated by the external waste treatment company.

Liquid samples are collected in a vessel (inlet funnel is in the fume hood) and emptied approximately every two weeks. This material is recycled to the tar refinery.

During the whole time spent in the laboratory, the laboratory technicians wear specific PPE:

- Lab coat or chemically resistant working clothes
- Safety glasses
- One time nitrile lab gloves (when handling product) (0.1 mm thickness)

Description of data used for assessment of workers' exposure

Regular biomonitoring campaigns are conducted at Rain Carbon. In the following, data obtained from campaigns through the years 2012-2018 on laboratory workers are reported.

Two types of measurements are available for laboratory staff:

- Campaigns measuring pre- and post-shift 1-OH pyrene levels in urine on day 1 and day 5 of the work week were taken.
- Post-shift measurements at randomly selected days.

Summary statistics and a description of methods are provided in a separate document. Workers are split according their smoking status (non-smokers and smokers).

Table 9-40: Number* of individual workers monitoring 2012 – 2018 (SD: shut-down periods, NO: normal operation)

Campaign		2012	2013	2014	2015	2016	2017	2018	Total
Day 1 – 5 full week	smokers	-	-	-	-	-	-	-	-
	non-smokers	3	-	-	-	-	-	-	3
Random sampling	smokers	-	-	-	-	-	-	-	-
	non-smokers	12	-	-	-	-	1	2	15
Total		15	-	-	-	-	1	2	18

* Only individuals with all 4 samples (i.e. day 1 and 5 pre- and post-shift) available were counted

In Table 9-41 arithmetic means and 90th percentiles for the two types of data for laboratory workers are presented.

Table 9-41: Results from biomonitoring campaigns 2012 – 2018; all values are given as 1-hydroxypyrene in urine [µg 1-OHP/g creatinine], measured on day 5, end of shift; non-smokers only)

Job description	n	AM	STD	90th percentile
Day 1 – 5 full week	3	0.27	0.21	0.44
Random sampling	15	0.39	0.35	0.56

The measured values are given with the unit µg 1-hydroxypyrene/g creatinine. These values are converted with the divisor 1.93 (molecular weight of 1-OHP of 218.26 g/mol, divided by molecular weight of creatinine of 113.12 g/mol) into values with the unit µmol/mol creatinine.

For converting this to a BaP workplace air concentration the equation as given in ECHA (according to 2018) is used:

BaP workplace air concentration [ng/m³] = ((1-OHP urinary concentration [µmol/mol creatinine] – 1.13)/11.1) x 1 000

In the following table 90th percentile values for the two types of measurements as shown in Table 9-41 are converted into BaP air concentrations.

Table 9-42: Transformation of 1-hydroxypyrene levels (90th percentiles) into BaP workplace air concentrations

Job description	1-OHP in urine [µg/g creatinine]	1-OHP in urine [µmol/mol creatinine]	Corresponding conc. of BaP in workplace air [ng/m³]
Day 1 – 5 full week	0.44	0.23	-
Random sampling	0.56	0.29	-

Discussion

The data in Table 9-42 show that on average workers in these groups have 1-OHP values below 0.4 µg/g creatinine and values below 0.6 µg/g creatinine at the 90th percentile level. These levels are in the background exposure range. Dhooge et al. (2010) report medians (with 10th-90th percentile ranges) for Flemish adult men and women of 0.135 (0.024-0.588) and 0.147 (0.041-0.73) µg/g creatinine, respectively. The above reported 90th percentile values are below those reported by Dhooge et al.

According to RACs exposure-risk relationship exposures with 1-OHP levels below 1.13 µmol/mol creatinine are not associated with a relevant workplace exposure.

Therefore it can be concluded that laboratory workers don't have relevant workplace-related exposures to PAHs.

Dermal exposure

The biomonitoring data above indicate that systemic exposure to PAHs at the laboratory workplaces is negligible. Therefore, it can also be concluded that dermal exposure is negligible, a result, which is expected due to the workplace situation and adequate PPE in use to avoid any exposure.

Conclusion on risk characterisation:

According to ECHA's Q&A Reference number: ID 0585 regarding the scope of the exemption from Authorisation of activities that might be considered to be falling under scientific research and development, analytical activities such as monitoring and quality control are outside the scope of authorisation, if carried out under controlled conditions in a volume less than one tonne per year. These conditions apply: the total amount of samples on formulations does not exceed 1 ton/year. Suitable technical and organisation measures as well as personal protection equipment are applied to ensure controlled conditions. We provide here a full exposure description and assessment, but – based on this exemption – refrain from calculating excess cancer risks for this contributing scenario. But the exposure

assessment above shows that exposure levels during handling in the laboratory are expected to be negligible.

9.1.5 Worker contributing scenario 3 – PROC 28 – Maintenance workers

9.1.5.1 Conditions of use

Table 9-43: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture: 50-99% CTPht in pitch mixtures • Physical form of the used product: liquid
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: ≤8 h/day
Technical and organisational conditions and measures
• Permit system for line opening • Emptying of lines before opening
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes, during specific tasks with potential dermal exposure such as dismounting of pumps • Respiratory Protection: Yes, during specific tasks with potential respiratory exposure such as dismounting of pumps • Eye protection: Yes, during specific tasks with potential exposure to eyes such as dismounting of pumps • Working clothes: Yes • Protection boots: Yes • Helmets: Yes
Other conditions affecting workers exposure
• Place of use: Outdoor • Operating temperature: ≤30 °C (in tasks related to potential exposure such as dismounting of pumps)

9.1.5.2 Exposure and risks for workers

The 21 maintenance workers at Rain Carbon only spend a small amount (0.55%) of their overall working time (21 x 1 530 h = 32 130 h) on maintenance activities related to the pitch mixtures. Approximately 96h per year they conduct maintenance tasks related to formulation equipment where exposure may be possible (based on records from maintenance procedures for formulation equipment), and 81 h per year they spend on ship loadings with pitch mixtures. In total, the maintenance workers conduct tasks related to pitch mixtures during 0.55% of their overall labour time (32 130/(96 + 81) x 100 = 0.55%). A rounded figure of 1% is used for risk characterisation.

Most of the maintenance cases are assigned to the distillation procedure on the tar refinery/manufacture as this process contains the most equipment where maintenance is

necessary. Regular maintenance related to pitch mixtures may only occur on pumps, valves or loading arms, which are activities where stringent procedures apply regarding cleaning and flushing prior to maintenance, ensuring that the equipment arrives clean in the workshop. Flushing/draining the equipment before disconnecting if from the process is performed by the logistics operator, after which the equipment is moved to the cleaning box, opened and cleaned by the maintenance staff (see below). Written procedures are available with detailed instructions on e.g. how to proceed in case that a pump needs to be repaired (close the lines, empty and clean the pump, transport the pump to the repair shop,…) or cleaned and what PPE has to be used. Specific activities where maintenance workers are involved in tasks related to pitch mixtures are:

Assisting the logistics operator during ship loading

(For a detailed description see section 9.1.3.2)

Maintenance on loading arms

The loading arms for the tank truck loading stations need maintenance from time to time. For instance, the joints need lubrication or some technical equipment may need to be repaired. In the latter case, the broken part is taken out, cleaned in the cleaning box (see below) and repaired in the workshop. These maintenance activities are conducted by the mechanical workshop team and occur approximately once every 12-24 months. Before mechanical works are initiated, the loading arm is drained and cleaned with high pressure water. This job typically takes one to two days with two workers.

Mechanical interventions on the closed lines/ dismounting of pumps

The plant operators prepare the system for intervention before the mechanical workshop takes over. The maintenance workers have a permitting system for several works, all EHS aspects are covered. Defective equipment needing internal repairs is typically removed from the plant, cleaned by the maintenance staff and then brought in the workshop for repairs.

External repairs (e.g.) exchange of the electrical motor, tension adjustment on flanges etc. can be done in the plant without removing the equipment. Maintenance work regarding mechanical interventions on the closed lines related to the formulation process is related to pump maintenance and occurs at 6-7 pumps/year.

When the system needs to be opened, e.g. in case a pump needs to be repaired, the lines are closed and emptied and the pump needs to be rinsed. For this, there are several possibilities. For pitch: the remaining liquid is pushed out of the pump with steam or nitrogen before the pump is dismounted. Any remains of the substance is left to cool down until it solidifies and discharged as hazardous waste.

All dismounted technical equipment is water-blasted and cleaned thoroughly from the in- and outside in the cleaning area before it is transported into the workshop, where it is disassembled and repaired. The workshop is equipped with several countertops, each provided with a LEV pipe from the ceiling, a mesh and all PPE necessary, including several types of different gloves, suitable for all kinds of operations.

Note that, in case of broken pumps, since all pumps are installed in double or triple and the backup takes over for a broken pump, there is no time pressure for the maintenance activity, which reduces the potential for contamination and allows the maintenance workers to approach things in the best possible way.

A typical maintenance procedure for pump replacement is:

- Setting all controls to safe position
- Drain/rinse/cool down
- Remove insulation
- Mechanical removal pump
- Installation of spare pump if necessary (in most positions 1 or 2 spare pumps/position are installed, a spare pump is in the warehouse to be able to switch in the field)
- Pump re-install
- Insulation + restart
- Afterwards :
    - Failed pump cleaning in cleaning box
    - Pump is serviced in the workshop and replaced in warehouse

Cleaning of dismounted technical equipment or pipes

All equipment cleaning is conducted by the maintenance workers within the dedicated cleaning box, which is equipped with a drainage for the cleaning water. It should be noted that the equipment arriving at the cleaning box of the maintenance shop has typically already been flushed, emptied and cleaned a first time when the part was removed (in order to not have to move a heavily contaminated part). A typical cleaning procedure takes approximately 1, during which the object is thoroughly cleaned with a water-jet from a lance. The cleaned object is then transported to the repair shop. In addition to the protection equipment described below, workers wear a chemically resistant/watertight coverall, gloves and a mask when necessary.

Tank opening – regular maintenance

There are no regular maintenance shutdowns for the formulation process, tanks only need to be opened or replaced after their lifetime (lifetime of a pitch tank >30 years). In these cases, the tanks are opened and emptied, demolished and replaced by new tanks. Due to the highly infrequent occurrence of this activity, it is not included in the quantitative exposure assessment.

Only in some cases, the tank has to be opened during its lifetime for structural integrity inspection (often required by law). In these cases, an underpressure is built in the tank and air is sent over particle filters. However, more and more alternative techniques are being developed that allow external measurement and which prevent to open the tank.

During these procedures, the maintenance worker wears specific PPE:

- Heavy duty nitrile rubber gloves, thickness 1.1 mm
- Full mask (in case they have to perform an operation that could lead to pitch vapours exposure), filter ABEK P3 Chemically resistant coverall
- Face shield
- Safety goggles

Respiratory protection (half or full masks with filters ABEK P3 are worn if there is potential for inhalation exposure.

Description of data used for assessment of workers' exposure

Regular biomonitoring campaigns are conducted at Rain Carbon. In the following Table 9-44, data obtained from campaigns through the years 2012-2018 are reported.

Table 9-44: Number* of individual maintenance workers monitoring 2012 – 2018 (SD: shut-down periods, NO: normal operations)

	2012	2013	2014	2015	2016	2017	2018	Total
Smokers SD	-	1	-	-	-	1	-	2
Non-smokers SD	-	3	-	-	-	-	-	3
Smokers NO	-	-	1	-	-	2	-	3
Non-smokers NO	**2**	**-**	**1**	**-**	**4**	**1**	**-**	**8**
Total	2	4	2	-	4	4	-	16

* Only individuals with all 4 samples (i.e. day 1 and 5 pre- and post-shift) available were counted

During these campaigns pre- and post-shift measurements on day 1 and day 5 of the work week were taken. A description of methods is provided in Annex XI and summary statistics are provided in a separate (confidential) document. Workers are split according to their smoking status (non-smokers and smokers). Also, values measured during general shutdown periods (5 out of 16 values) are not included. As explained above, general shutdowns do not relate to formulation activities, as these are not subject to annual maintenance activities. The remaining measurements were taken during normal production routines and include typical activities as described above for maintenance workers. Again, to eliminate the PAH contribution from smoking, only non-smokers were included in the assessment. The full dataset is documented in the separate document.

In the following, the exposure assessment is based on all measurements from 2012 to 2018 for non-smokers (normal operation, see in bold in table above) for values obtained end-of-shift on day 5.

In a conservative way the risk characterisation is based on 90th percentiles, although for calculating cancer risks the long-term average exposure is more relevant.

Table 9-45: Results from biomonitoring campaigns 2012 – 2018; all values are given as 1-hydroxypyrene in urine [µg 1-OHP/g creatinine], measured on day 5, end of shift; 90th percentile values used for risk characterisation (normal production, non-smokers only)

Job description	n	AM	STD	90th percentile
Maintenance workers	8	1.40	1.03	2.36

The measured values are given with the unit µg 1-hydroxypyrene/g creatinine. These values are converted with the divisor 1.93 (molecular weight of 1-OHP of 218.26 g/mol, divided by molecular weight of creatinine of 113.12 g/mol) into values with the unit µmol/mol creatinine.

For converting this to a BaP workplace air concentration the equation as given in ECHA (according to 2018) is used:

BaP workplace air concentration [ng/m^3] = ((1-OHP urinary concentration [µmol/mol creatinine] – 1.13)/11.1) x 1 000

In Table 9-46 the 90th percentile value for maintenance workers as shown in Table 9-45 is converted into a BaP air concentration.

Table 9-46: Transformation of 1-hydroxypyrene levels (90th percentiles) into BaP workplace air concentrations

Job description	1-OHP in urine [µg/g creatinine]	1-OHP in urine [µmol/mol creatinine]	Corresponding conc. of BaP in workplace air [ng/m^3]
Maintenance workers	2.36	1.22	8.39

Excess lifetime cancer risks per job description are calculated (Table 9-47) based on these 90th percentile values, taking into consideration the share of time spent on formulation activities and using the exposure-risk relationship as published by RAC (ECHA, 2018).

Table 9-47: Excess lifetime cancer risks (ELCRs) for maintenance workers (N = 21 workers)

Target organ:	Long-term exposure [ng BaP/m^3] *	% of time related to formulation	Corrected concentration [ng BaP/m^3]	Risk estimate for cancer per ng BaP/m^3 (40 years of occupational exposure)	ELCR
	8.39	1%	0.084		
Lung				5.60E-06	4.70E-7
Bladder				4.00E-06	3.36E-7
Combined					8.06E-7

* Based on 90th percentile biomonitoring values

Discussion

The data in Table 9-45 show that on average maintenance workers have 1-OHP values below 1.4 µg/g creatinine (or 0.73 µmol/mol creatinine). According to RACs exposure-risk relationship this relates to a negligible workplace exposure to PAH (1-OHP levels below 1.13 µmol/mol creatinine are not associated with an increased cancer risk due to workplace exposure).

At the 90th percentile levels exposure is just above the 1.13 µmol/mol creatinine level (90th percentile: 1.22 µmol/mol creatinine). The resulting theoretical excess cancer risk is slightly above 10^{-5} for each lung and bladder cancer and, when the low contribution from formulation activities is taken into account, the excess risk is below 10^{-6}, indicating very low risks.

Further, this risk calculation is very conservative: using the 90th percentile values for the risk characterisation means that it is assumed that each individual worker in whole group is exposed daily for 40 years at this level.

Dermal exposure

As explained above, for most activities dermal exposure is not possible, as the material are kept at temperatures as high as 230 °C and any contact would immediately cause severe burns.

For some specific activities contact cannot be completely dismissed, such as handling of contaminated objects. As explained above, all objects which are delivered to the repair shop, are thoroughly drained before entering in the cleaning box. Therefore, only residual contaminations, remain on the object. Contamination of surfaces would also be readily detected due to the black colour of all materials containing coal tar pitch. Workers in the repair shop are well instructed and have various protective equipment in place (various types of gloves suitable for specific tasks) to choose from.

In the following we intend to give a semi-quantitative impression on the relevance of dermal contact. To this end, two scenarios are developed.

We tried to apply dermal exposure modelling, but the available Tier II model RiskOfDerm does not contain a scenario for handling contaminated objects (this scenario was removed from a previous version due to poor data coverage and high uncertainties). We therefore developed an own scenario, based on the specific conditions at these workplaces.

The following assumptions are used to estimate the dermal exposure during handling of objects in the repair shop:

- during repair of an object (e.g. broken pump) a contamination of 10 cm^2 skin occurs (fingertips of both hands)
- the skin loading with mixture is assumed to be 0.1 mg/cm^2 (typical value for low-level contamination, see e.g. assumptions for EASE model in the Technical Guidance Document on Risk Assessment (EC, 2003b), assumed here for pre-cleaned objects)
- Total amount of BaP on skin is 10 cm^2 x 0.1 mg/cm^2 x 0.8% BaP in mixture (x 0.008) = 8 µg BaP/person/event

- Dermal absorption of PAH: 30% (according to EU Risk Assessment Report (ECB, 2008)): 2.4 µg BaP/person/event
- Glove protection factor 20 leads to a total dose of 0.12 µg BaP/person/event
- Frequency correction factor: activity performed once (conservative assumption) per year per worker: 0.12 µg BaP/person/event / 220 d/a = 0.55 ng BaP/person/day.

Comparison with uptake from inhalation at ambient background exposure concentrations

Total amount inhaled from background air exposure (see Table 9-23): 0.2 ng BaP/m^3 = 4 ng BaP/person/day (with 20 m^3 respiratory volume per day and 100% absorption assumed).

The scenario described above results in a total amount of BaP taken up, which is lower by factor 7 compared to the amount taken up from inhaling ambient air with typical background concentrations of BaP (based on annual averages). Although this scenario includes high uncertainties, together with practical experience from the workplace situation, it is concluded that dermal exposure is negligible for the situations described, due to

- hygiene conditions (thorough cleaning)
- consequent application of personal protection equipment
- and rare contact with potentially contaminated objects.

Conclusion on risk characterisation:

Calculated extra cancer risk for maintenance workers (21 workers) is 8.06 x 10^{-7}.

10 RISK CHARACTERISATION RELATED TO COMBINED EXPOSURE

10.1 Human health (related to combined exposure)

10.1.1 Workers

Use 1A/B

The WCS for the uses described in this CSR address the different groups of workers separately. Exposures and calculated cancer risks are given per group, based on estimated long-term shift average concentrations of BaP. No combined exposure from different WCS occurs.

No overlap exists between the workers in the two different uses. Workers exposure is not relevant for use 1B (anthracene oil).

10.1.2 Consumers

There is no consumer use of CTPht or AO.

10.2 Environment (combined for all emission sources)

10.2.1 All uses (regional scale)

Exposure from Use 1A/B comes from one specific site in northern Belgium.

10.2.2 Local exposure due to all wide dispersive uses

There are no wide dispersive uses of CTPht and AO.

10.2.3 Local exposure due to combined uses at a site

For formulation activities combined exposures from CTPht and AO were considered and discussed in section 9.1.

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12 ANNEX I – SITE MAPS

Figure: **Schematic site-map of Rain Carbon with tar refinery (red box)**

Figure: **Site-map of Rain Carbon and surroundings**

13 ANNEX II – OFFICIAL REAEASE PERMITS (WATER) FOR THE 16 EPA PAHS

Table: Official release permits for step-wise decrease of 16 EPA PAH emissions to water

PAHs	>2011 [µg/L]	>2014 [µg/L]	>2019 [µg/L]
Naphthalene	40.00	20.00	20.00
Acenaphthylene	65.00	65.00	65.00
Acenaphthene	38.00	38.00	38.00
Fluorene	25.00	25.00	25.00
Anthracene	2.00	0.40	0.40
Phenanthrene	13.00	13.00	13.00
Fluoranthene	5.00	1.00	1.00
Pyrene	6.90	1.60	1.22
Benz[a]anthracene	2.40	1.20	1.20
Chrysene	2.00	0.70	0.70
Benzo[a]pyrene	0.50	0.50	0.50
Benzo[b]fluoranthene	2.60	0.51	0.48
Benzo[k]fluoranthene	2.60	0.52	0.44
Benzo[ghi]perylene	1.20	0.50	0.47
Dibenz[a,h]anthracene	0.30	0.14	0.14
Indeno[1,2,3-cd]pyrene	0.70	0.28	0.26
Sum of 16 EPA PAHs	207.20	168.35	167.81

14 ANNEX III – PAH EMISSIONS FROM THE FOUR RELEVANT SCRUBBERS – RAW DATA FROM 2009 TO 2018

Table: PAH emissions from the four relevant scrubbers [kg/year] – raw data for 2009, 2012 and 2018

	K101			K102			K100A			31B101			Sum of all 4 scrubbers		
	2009	2012	2018	2009	2012	2018	2009	2012	2018	2009	2012	2018	2009	2012	2018
Naphthalene	< 0.2630	0.9121	0.0813	< 0.0001	1.3341	1.8712	12.1760	0.0062	0.4212	30.4850	1.0382	0.0029	< 42.9241	3.2906	2.3765
Acenaphthylene	< 0.0090	0.0045	0.0025	< 0.0001	0.0124	0.0409	0.3680	0.0002	0.0100	1.2180	0.0058	0.0002	< 1.5951	0.0229	0.0536
Acenaphthene	< 0.1660	0.2499	0.0788	0.0001	0.8672	3.2258	7.0960	0.0010	4.8175	30.4850	0.4038	0.0263	< 37.7471	1.5219	8.1484
Fluorene	< 0.0610	0.0052	0.0011	< 0.0001	0.0162	0.5909	0.1140	0.0002	0.0038	1.3050	0.0044	0.0018	< 1.4801	0.0260	0.5975
Anthracene	0.0260	0.0066	< 0.0011	< 0.0001	0.0070	0.0106	< 0.0001	< 0.0000	0.0013	0.5780	0.0011	0.0002	< 0.6042	< 0.0147	< 0.0132
Phenanthrene	< 0.0260	0.0400	0.0054	0.0090	0.0362	1.1595	0.0790	0.0002	0.0035	3.1890	0.0069	0.0026	< 3.3030	0.0833	1.1710
Fluoranthene	0.0000	0.0175	0.0014	< 0.0090	0.0172	0.5789	0.0090	0.0000	0.0032	0.5780	0.0021	0.0004	< 0.5960	0.0368	0.5839
Pyrene	0.0000	0.0092	0.0006	0.0001	0.0105	0.5729	< 0.0001	< 0.0000	0.0019	0.2890	0.0011	0.0002	< 0.2892	< 0.0208	0.5756
Benzo[a]anthracene	< 0.0000	0.0003	0.0001	< 0.0001	0.0009	0.0029	0.0001	0.0002	0.0014	< 0.0001	0.0002	0.0000	< 0.0003	0.0016	0.0044
Chrysene	< 0.0000	0.0003	< 0.0001	< 0.0001	0.0009	0.0021	< 0.0001	< 0.0002	0.0007	< 0.0001	< 0.0002	0.0000	< 0.0003	< 0.0016	< 0.0029
Benzo[a]pyrene	< 0.0000	< 0.0001	< 0.0001	< 0.0001	0.0001	0.0002	< 0.0001	< 0.0002	0.0005	< 0.0001	< 0.0002	< 0.0000	< 0.0003	< 0.0006	< 0.0008
Benzo[b]fluoranthene	< 0.0000	0.0001	< 0.0001	< 0.0001	0.0002	0.0005	0.0001	< 0.0002	0.0010	0.0001	0.0002	0.0000	< 0.0003	< 0.0007	< 0.0016
Benzo[k]fluoranthene	< 0.0000	< 0.0001	0.0001	< 0.0001	< 0.0001	0.0002	< 0.0001	< 0.0002	0.0002	< 0.0001	< 0.0002	< 0.0000	< 0.0003	< 0.0006	< 0.0005
Benzo[ghi]perylene	0.0000	< 0.0001	< 0.0001	0.0090	< 0.0001	< 0.0001	0.0001	0.0002	0.0001	< 0.0001	< 0.0002	< 0.0000	< 0.0092	< 0.0006	< 0.0003
Dibenzo[a,h]anthrancene	< 0.0000	< 0.0001	< 0.0001	< 0.0001	< 0.0001	0.0000	< 0.0001	< 0.0002	0.0001	< 0.0001	< 0.0002	< 0.0000	< 0.0003	< 0.0006	< 0.0002
Indeno[1,2,3-cd]pyrene	< 0.0000	< 0.0001	< 0.0001	< 0.0001	< 0.0001	0.0001	< 0.0001	< 0.0002	0.0004	< 0.0001	0.0002	0.0000	< 0.0003	< 0.0006	< 0.0006
EPA PAH (sum 16)	0.5518	< 1.2462	< 0.1727	0.0280	< 2.3032	8.0567	< 19.8429	< 0.0095	5.2669	< 68.1276	1.4649	< 0.0347	< 88.5501	< 5.0239	< 13.5312

PAHs relevant for PBT assessment (sum 9)	0.0520	< 0.0742	< 0.0090	< 0.0276	0.0730	2.3272	0.0887	< 0.0012	0.0128	< 4.6345	< 0.0122	0.0036	< 4.8028	< 0.1606	< 2.3526
4 EFSA PAHs relevant for assessment of HvE (sum 4)	0.0000	0.0008	0.0004	0.0004	0.0021	0.0057	0.0004	0.0008	0.0036	0.0004	0.0008	0.0001	0.0012	0.0045	0.0097
Flow (Nm^3/hour)	<75	14	20 [1]	<75	11	20 [1]	88	24	14 [2]	79	21	25			
Possible scaling factors	51% of the time fully open, 23% of the time fully closed			2% of the time fully open, 73 % of the time fully closed			67% of the tank farm volume contains AFA formulations with AO.								
PAH reduction program planned actions	2019: post-treatment on activated carbon (> 80% yield)			2019: post-treatment on activated carbon (>80% yield)			2019: connection to thermal incinerator of the tar refinery (99-100% yield)			2019: post-treatment on activated carbon (> 80% yield)					

[1] Flowrates below the measuring range of the equipment have been determined using process data.

[2] Average 2018 flowrate.

15 ANNEX IV – EFFICIENCY OF PAH ADSORPTION ON ACTIVE CARBON

1) Literature on the adsorption of PAH on active carbon

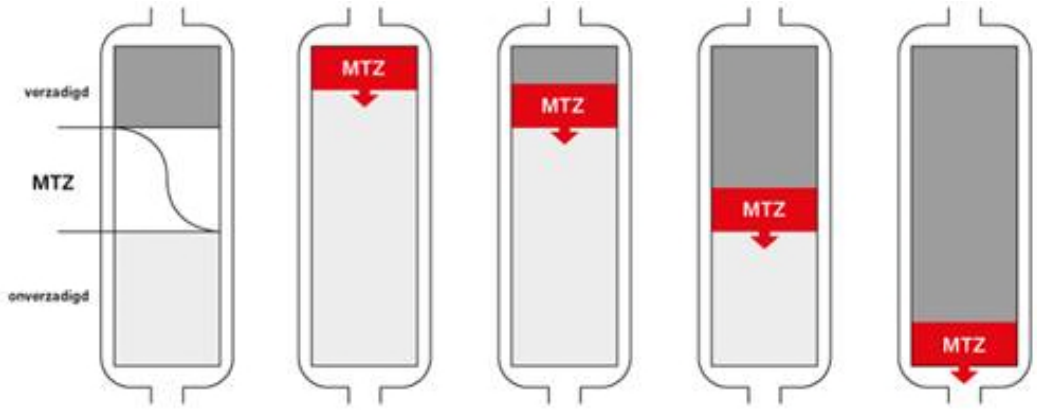
Articles: Measurements of polycyclic aromatic hydrocarbon adsorption on activated carbons at very low concentrations (Mastral et al., 2003)

Adsorption of phenanthrene on activated carbons: Breakthrough curve modeling (Murillo et al., 2004)

These articles mention the adsorptions isotherms of PAH (poly aromatic hydrocarbons) on active carbon. Before the breakthrough time 100% of the PAH are adsorbed. For 2 ppm phenanthrene at a flowrate of 10 mL/min the breakthrough time was 7-18 h on an active carbon bed of 25 mg.

2) Supplier of active carbon

Desotec delivers active carbon "Airpel super 4 and Airpel 10" for the 1.5-4 m³ fixed bed filters on our site. PAHs are easily adsorbed on active carbon, the heavier components better than the lighter.



Based on the evaluation of the process conditions (concentrations and flow) of our scrubbers, using the right bed volume for the flow rate, desotec calculates the removal efficiency to be >99%. On breakthrough the active carbon has to be exchanged.

3) Other literature

Article: Experimental study on the removal of PAHs using in-duct activated carbon injection (Zhou et al., 2005)

This article mention a removal efficiency of 91% at 2 g active carbon /Nm³ injection in the flue gasses of an incinerator. However at our site we use active carbon in a fixed bed filter, which has higher efficiency. We do not inject it in flue gasses.

16 ANNEX V – PAH EMISSIONS FROM THE FOUR RELEVANT SCRUBBERS – EMISSIONS FROM 2009 AND APPLIED REDUCTION FACTORS

Table: PAH emissions from the four relevant scrubbers – emissions from 2009 and applied reduction factors [kg/y]

	K101		K102		K100A		31B101		Sum of all 4 scrubbers	
	Emission [a]	Emission reduced by 80% [b]	Emission [a]	Emission reduced by 80% [b]	Emission [a]	Emission reduced by 99% [c]	Emission [a]	Emission reduced by 80% [b]	Emissions [a]	Reduced emissions
Anthracene	1.30E-02	2.60E-03	4.00E-05	8.00E-06	4.50E-05	4.50E-07	5.78E-01	1.16E-01	5.91E-01	1.18E-01
Phenanthrene	1.30E-02	2.60E-03	4.50E-03	9.00E-04	7.90E-02	7.90E-04	3.19E+00	6.38E-01	3.29E+00	6.42E-01
Fluoranthene	4.00E-05	8.00E-06	4.50E-03	9.00E-04	9.00E-03	9.00E-05	5.78E-01	1.16E-01	5.92E-01	1.17E-01
Pyrene	4.00E-05	8.00E-06	4.00E-05	8.00E-06	4.50E-05	4.50E-07	2.89E-01	5.78E-02	2.89E-01	5.78E-02
Benzo[a]anthracene	4.00E-05	8.00E-06	4.00E-05	8.00E-06	4.50E-05	4.50E-07	4.00E-05	8.00E-06	1.65E-04	2.45E-05
Chrysene	4.00E-05	8.00E-06	4.00E-05	8.00E-06	4.50E-05	4.50E-07	4.00E-05	8.00E-06	1.65E-04	2.45E-05
Benzo[a]pyrene	4.00E-05	8.00E-06	4.00E-05	8.00E-06	4.50E-05	4.50E-07	4.00E-05	8.00E-06	1.65E-04	2.45E-05
Benzo[b]fluoranthene	4.00E-05	8.00E-06	4.00E-05	8.00E-06	4.50E-05	4.50E-07	4.00E-05	8.00E-06	1.65E-04	2.45E-05
Benzo[k]fluoranthene	4.00E-05	8.00E-06	4.00E-05	8.00E-06	4.50E-05	4.50E-07	4.00E-05	8.00E-06	1.65E-04	2.45E-05
Benzo[ghi]perylene	4.00E-05	8.00E-06	4.50E-03	9.00E-04	4.50E-05	4.50E-07	4.00E-05	8.00E-06	4.63E-03	9.16E-04
9 PAHs relevant for PBT assessment	2.63E-02	5.26E-03	1.37E-02	2.75E-03	8.83E-02	8.83E-04	4.63E+00	9.27E-01	4.76E+00	9.36E-01

[a] In case that the emission was provided with "<" in the raw data table (see table above), the given value was divided by 2 (considering LOD/2 for the measured concentration).

[b] A conservative reduction of 80% was applied to the emission value since emission from this scrubber will be post-treated on activated carbon from end of 2019 onwards and a yield of >80% removal is expected.

[c] A conservative reduction of 99% was applied to the emission value since emission from this scrubber will be post-treated on activated carbon from end of 2019 onwards and a yield of 99-100% removal is expected.

17 ANNEX VI – EMISSIONS TO WATER FOR 2001-2018

Table: Total PAH emissions to water and discharge volumes per year for 2001-2018

Total emission per year [mg/day]																		
PAHs	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018
Anthracene	96.0	126.8	167.7	37.5	80.8	133.3	130.3	134.0	37.4	68.9	93.6	47.1	32.8	3.5	10.6	11.6	18.0	16.8
Phenanthrene	560.5	411.3	819.8	139.8	261.6	69.4	133.3	147.7	232.3	230.6	177.3	17.8	16.8	12.8	16.2	31.9	65.0	68.7
Fluoranthene	376.9	544.3	587.7	186.2	192.1	196.9	269.1	338.0	163.8	281.3	195.1	22.6	21.2	8.3	13.6	95.7	53.2	55.1
Pyrene	248.5	307.2	554.7	159.9	98.7	151.3	184.1	224.6	133.0	161.4	126.8	11.5	12.5	4.1	6.6	61.8	29.6	25.8
Benzo[a]anthracene	42.8	80.6	84.9	58.0	56.0	60.3	68.5	79.0	58.9	62.9	38.4	2.0	7.5	2.2	1.4	20.0	11.9	15.2
Chrysene	72.0	52.6	56.4	49.4	184.2	56.2	64.5	81.2	51.1	56.0	32.4	2.5	5.4	6.7	2.1	22.4	19.9	18.9
Benzo[a]pyrene	27.2	30.4	25.1	21.4	13.0	25.9	32.6	35.4	24.1	69.9	23.4	3.6	7.0	3.8	1.3	16.1	16.4	11.1
Benzo[b]fluoranthene	29.8	35.1	40.9	26.8	18.3	34.3	48.8	50.8	30.2	38.5	26.1	2.3	8.3	5.1	2.3	32.8	31.8	23.4
Benzo[k]fluoranthene	7.8	20.4	18.1	22.0	11.8	18.5	18.6	24.3	18.6	24.1	16.0	1.9	5.6	2.6	2.1	12.0	13.0	12.6
Benzo[ghi]perylene	12.3	10.0	8.2	7.7	7.3	12.4	17.1	14.6	12.7	19.2	7.5	0.9	2.1	0.6	1.0	11.0	13.6	10.2
9 PAHs relevant for PBT assessment	1456.4	1593.7	2330.9	689.7	912.9	736.5	935.4	1093.3	744.6	993.5	717.9	110.5	113.0	45.2	55.9	293.5	254.2	244.6
Discharge volume [m^3/year]	71 034 [a]	71 034 [a]	71 034	76 325	92 637	85 980	90 853	89 218	92 201	131 400	97 245	111 206	122 377	118 242	101 183	101 231	109 413	109 413 [b]

[a] Discharge volume estimated according to the discharge volume of 2003.

[b] Discharge volume estimated according to the discharge volume of 2017.

The data are means of approximately 100 measurements per year (for 2017 and 2018, for the years before 2017 no information is available about the number of measurements per year).

18 ANNEX VII – SALINITY OF THE CANAL CLOSE TO THE PLANT

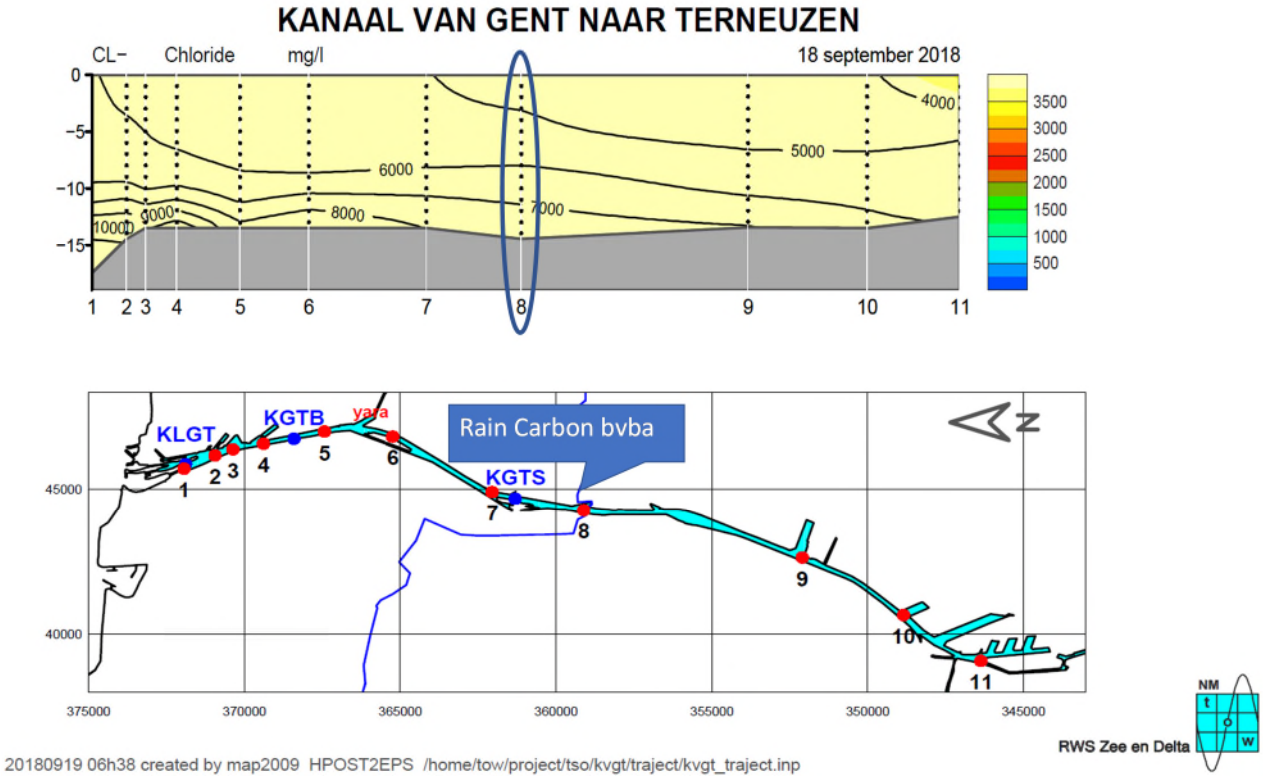


Figure: Salinity of the canal close to the plant

The salinity at point 8 is between ~4 000 and ~7 500 mg/L, which corresponds to 0.4-0.75%. Accordingly, the water in the canal close to the plant and to the measuring point MP 30000 is brackish water.

19 ANNEX VIII – BELGIAN FOOD CONSUMPTION DATA

Table: Consumption of the five EUSES food categories representative for the Belgian population

	Male, 18-39	Female, 18-39	Male, 40-64	Female, 40-64	MEAN	MAX	Unit
	N = 305	N = 315	N = 284	N = 322			
Root crops *							
Potatos and other root crops	74	52	83	57	**67**	83	[g/day]
EUSES default for root crops	384	384	384	384	384	384	[g/day]
Consumption as % of default	19%	14%	22%	15%	17%	22%	[%]
Leaf crops *							
Vegetables	131	137	155	174	149	174	[g/day]
Leguminous plants	NA1	NA1	NA1	NA1			[g/day]
Fruits, nuts and olives	86	107	117	139	112	139	[g/day]
Cereals and cereal products	246	171	202	144	191	246	[g/day]
Confectionary and cakes	45	43	39	36	41	45	[g/day]
Sum	508	458	513	493	**493**	513	[g/day]
EUSES default for leaf crops	1 200	1 200	1 200	1 200	1 200	1 200	[g/day]
Consumption as % of default	42%	38%	43%	41%	41%	43%	[%]
Dairy products *							
Dauiry products and substitutes	196	183	168	199	**187**	199	[g/day]
EUSES default for dairy products	561	561	561	561	561	561	[g/day]
Consumption as % of default	35%	33%	30%	35%	33%	35%	[%]
Meat *							
Meat and meat products	145	95	145	98	121	145	[g/day]
Eggs and egg-derived products	12	8	14	8	11	14	[g/day]
Fats and oils	18	14	25	17	19	25	[g/day]
Sum	175	117	184	123	**150**	184	[g/day]
EUSES default for meat	301	301	301	301	301	301	[g/day]
Consumption as % of default	58%	39%	61%	41%	50%	61%	[%]
Fish *							

Fish and seafood	23	18	31	23	**24**	31	[g/day]
EUSES default for fish	115	115	115	115	115	115	[g/day]
Consumption as % of default	20%	16%	27%	20%	21%	27%	[%]
Total consumption of all groups acc. to survey	976	828	979	895	920	979	[g/day]
Total consumption of all groups acc. to EUSES	2 561	2 561	2 561	2 561	2 561	2 561	[g/day]

* Mean values were used.

Source: 2014-2015 National Food Consumption Survey, Belgium.

Weighted averages and percentiles for age, sex, season, and day of the week.

NA1 = not available due to too few people having consumed these foods during the two-day recall.

N = total number of people in the sample.

20 ANNEX IX – EUSES PROTOCOLS FOR THE TEN RELEVANT PAHS

20.1 Anthracene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Anthracene		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	8597AB55		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Anthracene		S
Description			D
CAS-No	120-12-7		S
EC-notification no.			D
EINECS no.	204-371-1		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	178.23	[g.mol-1]	S
Melting point	216.4	[oC]	S
Boiling point	342	[oC]	S
Vapour pressure at test temperature	9.40E-04	[Pa]	S
Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	9.40E-04	[Pa]	O
Octanol-water partition coefficient	4.68	[log10]	S
Water solubility at test temperature	47	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	0.047	[mg.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	2.95E+04	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	4.3	[Pa.m3.mol-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	580	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	4.97E+03	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	4.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	1.44E-06	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	1.30E-10	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	4.42E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			

INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	1.99E-05	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	7.15E-11	[mg.l-1]	O
Regional PEC in seawater (total)	6.74E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	6.81E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	6.61E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.18E-12	[mg.m-3]	O
Regional PEC in agricultural soil (total)	1.01E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.94E-12	[mg.l-1]	O
Regional PEC in natural soil (total)	1.17E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	1.17E-09	[mg.kgwwt-1]	O

Regional PEC in sediment (total)	8.55E-08	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	7.98E-09	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	2.47E-15	[mg.l-1]	O
Continental PEC in seawater (total)	3.22E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	2.36E-15	[mg.l-1]	O
Continental PEC in seawater (dissolved)	3.16E-15	[mg.l-1]	O
Continental PEC in air (total)	1.74E-15	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.49E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.86E-15	[mg.l-1]	O
Continental PEC in natural soil (total)	1.72E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.72E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.96E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	3.81E-12	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	4.17E-16	[mg.l-1]	O
Moderate PEC in water (dissolved)	4.09E-16	[mg.l-1]	O
Moderate PEC in air (total)	8.69E-18	[mg.m-3]	O
Moderate PEC in soil (total)	8.60E-15	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	4.94E-13	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	3.14E-16	[mg.l-1]	O
Arctic PEC in water (dissolved)	3.07E-16	[mg.l-1]	O
Arctic PEC in air (total)	1.93E-18	[mg.m-3]	O
Arctic PEC in soil (total)	6.42E-15	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	3.72E-13	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.19E-16	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.17E-16	[mg.l-1]	O
Tropic PEC in air (total)	3.36E-18	[mg.m-3]	O
Tropic PEC in soil (total)	1.75E-15	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	1.40E-13	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.476	[%]	O
Steady-state mass fraction in regional seawater	0.0499	[%]	O
Steady-state mass fraction in regional air	0.0884	[%]	O
Steady-state mass fraction in regional agricultural soil	15.3	[%]	O
Steady-state mass fraction in regional natural soil	1.99	[%]	O
Steady-state mass fraction in regional industrial soil	0.737	[%]	O
Steady-state mass fraction in regional freshwater sediment	6.56	[%]	O
Steady-state mass fraction in regional seawater sediment	0.204	[%]	O

CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.44E-03	[%]	O
Steady-state mass fraction in continental seawater	4.17	[%]	O
Steady-state mass fraction in continental air	0.0226	[%]	O
Steady-state mass fraction in continental agricultural soil	1.97	[%]	O
Steady-state mass fraction in continental natural soil	0.256	[%]	O
Steady-state mass fraction in continental industrial soil	0.0949	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.0199	[%]	O
Steady-state mass fraction in continental seawater sediment	0.853	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	30.1	[%]	O
Steady-state mass fraction in moderate air	1.25E-03	[%]	O
Steady-state mass fraction in moderate soil	0.0528	[%]	O
Steady-state mass fraction in moderate sediment	1.23	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	14.8	[%]	O
Steady-state mass fraction in arctic air	1.52E-04	[%]	O
Steady-state mass fraction in arctic soil	0.0172	[%]	O
Steady-state mass fraction in arctic sediment	0.606	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	19.6	[%]	O
Steady-state mass fraction in tropic air	7.93E-04	[%]	O
Steady-state mass fraction in tropic soil	0.0105	[%]	O
Steady-state mass fraction in tropic sediment	0.8	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	2.57E-04	[kg]	O
Steady-state mass in regional seawater	2.70E-05	[kg]	O
Steady-state mass in regional air	4.78E-05	[kg]	O
Steady-state mass in regional agricultural soil	8.25E-03	[kg]	O
Steady-state mass in regional natural soil	1.07E-03	[kg]	O
Steady-state mass in regional industrial soil	3.98E-04	[kg]	O
Steady-state mass in regional freshwater sediment	3.54E-03	[kg]	O
Steady-state mass in regional seawater sediment	1.10E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	7.79E-07	[kg]	O
Steady-state mass in continental seawater	2.25E-03	[kg]	O
Steady-state mass in continental air	1.22E-05	[kg]	O
Steady-state mass in continental agricultural soil	1.06E-03	[kg]	O
Steady-state mass in continental natural soil	1.38E-04	[kg]	O

Steady-state mass in continental industrial soil	5.13E-05	[kg]	O
Steady-state mass in continental freshwater sediment	1.07E-05	[kg]	O
Steady-state mass in continental seawater sediment	4.61E-04	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0162	[kg]	O
Steady-state mass in moderate air	6.78E-07	[kg]	O
Steady-state mass in moderate soil	2.85E-05	[kg]	O
Steady-state mass in moderate sediment	6.64E-04	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	8.00E-03	[kg]	O
Steady-state mass in arctic air	8.21E-08	[kg]	O
Steady-state mass in arctic soil	9.28E-06	[kg]	O
Steady-state mass in arctic sediment	3.27E-04	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0106	[kg]	O
Steady-state mass in tropic air	4.28E-07	[kg]	O
Steady-state mass in tropic soil	5.68E-06	[kg]	O
Steady-state mass in tropic sediment	4.32E-04	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	9.02E-08	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	6.31E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	6.31E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.86E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	6.30E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	6.30E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.86E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.60E-06	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.63E-06	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	3.17E-06	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	2.77E-09	[mg.l-1]	O
Local PEC in pore water of grassland	5.36E-09	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	2.77E-09	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			

MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D

EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D

NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D
MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D

INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D

DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S
BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	1	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.1	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	1	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	10	[-]	S
PNEC for marine organisms	0.1	[ug.l-1]	O

STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (fresh)	14	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	100	[-]	S
PNEC for fresh-water sediment organisms (from toxicological data)	0.14	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	0.295	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	No		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	0.28	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.14	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	14	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	1000	[-]	S
PNEC for marine sediment organisms (from toxicological data)	0.014	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.295	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	No		S
PNEC for marine sediment, normalised to 10% o.c. (local)	0.028	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.014	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	6.3	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	50	[-]	S
PNEC for terrestrial organisms (from toxicological data)	0.126	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.059	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	No		S
PNEC for terrestrial organisms	0.126	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O

RISK CHARACTERIZATION			
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	6.31E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	6.30E-03	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	6.65E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	0.0665	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	1.27E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	6.81E-07	[-]	O
RCR for the regional marine compartment	6.61E-08	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	2.81E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	2.62E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	9.09E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

20.2 Phenanthrene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Phenanthrene		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	796C7272		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Phenanthrene		S
Description			D
CAS-No	85-01-8		S
EC-notification no.			D
EINECS no.	201-581-5		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	178.23	[g.mol-1]	S
Melting point	100.5	[oC]	S
Boiling point	340	[oC]	S
Vapour pressure at test temperature	0.026	[Pa]	S
Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	0.026	[Pa]	O
Octanol-water partition coefficient	4.57	[log10]	S
Water solubility at test temperature	974	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	974	[ug.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	2.29E+04	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	3.7	[Pa.m3.mol-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	450	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	4.75E+03	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	4.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	1.44E-06	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	3.10E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	4.42E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S

Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	3.32E-05	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	1.18E-04	[ug.m-3]	O
Regional PEC in seawater (total)	1.22E-11	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.14E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	1.20E-11	[mg.l-1]	O

Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.58E-11	[mg.m-3]	O
Regional PEC in agricultural soil (total)	8.13E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	2.01E-11	[mg.l-1]	O
Regional PEC in natural soil (total)	9.28E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	9.28E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	1.10E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	1.11E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	9.32E-14	[mg.l-1]	O
Continental PEC in seawater (total)	3.08E-14	[mg.l-1]	O
Continental PEC in surface water (dissolved)	8.97E-14	[mg.l-1]	O
Continental PEC in seawater (dissolved)	3.03E-14	[mg.l-1]	O
Continental PEC in air (total)	8.71E-14	[mg.m-3]	O
Continental PEC in agricultural soil (total)	4.48E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.11E-13	[mg.l-1]	O
Continental PEC in natural soil (total)	5.11E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	5.11E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	8.69E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	2.80E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	4.01E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	3.94E-15	[mg.l-1]	O
Moderate PEC in air (total)	8.24E-16	[mg.m-3]	O
Moderate PEC in soil (total)	4.84E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	3.64E-12	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	2.92E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	2.88E-15	[mg.l-1]	O
Arctic PEC in air (total)	1.07E-16	[mg.m-3]	O
Arctic PEC in soil (total)	2.14E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	2.66E-12	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.09E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.07E-15	[mg.l-1]	O
Tropic PEC in air (total)	1.50E-16	[mg.m-3]	O
Tropic PEC in soil (total)	4.54E-14	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	9.88E-13	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			

REGIONAL			
Steady-state mass fraction in regional freshwater	0.0872	[%]	O
Steady-state mass fraction in regional seawater	0.01	[%]	O
Steady-state mass fraction in regional air	0.131	[%]	O
Steady-state mass fraction in regional agricultural soil	13.6	[%]	O
Steady-state mass fraction in regional natural soil	1.75	[%]	O
Steady-state mass fraction in regional industrial soil	0.647	[%]	O
Steady-state mass fraction in regional freshwater sediment	0.935	[%]	O
Steady-state mass fraction in regional seawater sediment	0.0314	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	6.02E-03	[%]	O
Steady-state mass fraction in continental seawater	4.43	[%]	O
Steady-state mass fraction in continental air	0.125	[%]	O
Steady-state mass fraction in continental agricultural soil	6.55	[%]	O
Steady-state mass fraction in continental natural soil	0.841	[%]	O
Steady-state mass fraction in continental industrial soil	0.312	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.0646	[%]	O
Steady-state mass fraction in continental seawater sediment	0.694	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	32	[%]	O
Steady-state mass fraction in moderate air	0.0132	[%]	O
Steady-state mass fraction in moderate soil	0.328	[%]	O
Steady-state mass fraction in moderate sediment	1	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	15.3	[%]	O
Steady-state mass fraction in arctic air	9.31E-04	[%]	O
Steady-state mass fraction in arctic soil	0.0633	[%]	O
Steady-state mass fraction in arctic sediment	0.48	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	19.9	[%]	O
Steady-state mass fraction in tropic air	3.92E-03	[%]	O
Steady-state mass fraction in tropic soil	0.0303	[%]	O
Steady-state mass fraction in tropic sediment	0.623	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	4.25E-04	[kg]	O
Steady-state mass in regional seawater	4.88E-05	[kg]	O
Steady-state mass in regional air	6.39E-04	[kg]	O

Steady-state mass in regional agricultural soil	0.0664	[kg]	O
Steady-state mass in regional natural soil	8.52E-03	[kg]	O
Steady-state mass in regional industrial soil	3.16E-03	[kg]	O
Steady-state mass in regional freshwater sediment	4.56E-03	[kg]	O
Steady-state mass in regional seawater sediment	1.53E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	2.94E-05	[kg]	O
Steady-state mass in continental seawater	0.0216	[kg]	O
Steady-state mass in continental air	6.10E-04	[kg]	O
Steady-state mass in continental agricultural soil	0.032	[kg]	O
Steady-state mass in continental natural soil	4.10E-03	[kg]	O
Steady-state mass in continental industrial soil	1.52E-03	[kg]	O
Steady-state mass in continental freshwater sediment	3.15E-04	[kg]	O
Steady-state mass in continental seawater sediment	3.38E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.156	[kg]	O
Steady-state mass in moderate air	6.43E-05	[kg]	O
Steady-state mass in moderate soil	1.60E-03	[kg]	O
Steady-state mass in moderate sediment	4.90E-03	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0745	[kg]	O
Steady-state mass in arctic air	4.54E-06	[kg]	O
Steady-state mass in arctic soil	3.09E-04	[kg]	O
Steady-state mass in arctic sediment	2.34E-03	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0973	[kg]	O
Steady-state mass in tropic air	1.91E-05	[kg]	O
Steady-state mass in tropic soil	1.48E-04	[kg]	O
Steady-state mass in tropic sediment	3.04E-03	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	4.89E-07	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.06E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	1.06E-07	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	2.44E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.06E-06	[mg.l-1]	O

Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.06E-06	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.43E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	8.50E-06	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	8.66E-06	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.67E-05	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.89E-08	[mg.l-1]	O
Local PEC in pore water of grassland	3.65E-08	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.89E-08	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D

Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D

NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D
MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S

BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	13	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	1.3	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	13	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	10	[-]	S
PNEC for marine organisms	1.3	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (fresh)	50	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	10	[-]	S
PNEC for fresh-water sediment organisms (from toxicological data)	5	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	2.98	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	No		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	10	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	5	[mg.kgdwt-1]	O

MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	50	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	10	[-]	S
PNEC for marine sediment organisms (from toxicological data)	5	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	2.98	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	No		S
PNEC for marine sediment, normalised to 10% o.c. (local)	10	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	5	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	18	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	10	[-]	S
PNEC for terrestrial organisms (from toxicological data)	1.8	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.596	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	No		S
PNEC for terrestrial organisms	1.8	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	8.18E-05	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	8.17E-04	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O

SEDIMENT			
RCR for the local fresh-water sediment compartment	2.44E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	2.43E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	4.72E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	8.75E-08	[-]	O
RCR for the regional marine compartment	9.23E-09	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	1.01E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	1.02E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	5.12E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

20.3 Fluoranthene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	Afa RainCarbon Fluoranthene		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	AB0FC50B		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Fluoranthene		S
Description			D
CAS-No	206-44-0		S
EC-notification no.			D
EINECS no.	205-912-4		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	202.25	[g.mol-1]	S
Melting point	108.8	[oC]	S
Boiling point	375	[oC]	S
Vapour pressure at test temperature	1.20E-03	[Pa]	S
Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	1.20E-03	[Pa]	O
Octanol-water partition coefficient	5.2	[log10]	S
Water solubility at test temperature	200	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	200	[ug.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	9.77E+04	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	1.1	[Pa.m3.mol-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	1.90E+03	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	2.77E+03	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	4.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	5.00E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			

Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	3.97E-05	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	2.07E-04	[ug.m-3]	O
Regional PEC in seawater (total)	1.99E-11	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.80E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O

Regional PEC in seawater (dissolved)	1.90E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	2.29E-12	[mg.m-3]	O
Regional PEC in agricultural soil (total)	2.14E-08	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.24E-11	[mg.l-1]	O
Regional PEC in natural soil (total)	2.38E-08	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	2.38E-08	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	7.59E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	7.90E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	3.15E-14	[mg.l-1]	O
Continental PEC in seawater (total)	1.46E-14	[mg.l-1]	O
Continental PEC in surface water (dissolved)	2.74E-14	[mg.l-1]	O
Continental PEC in seawater (dissolved)	1.39E-14	[mg.l-1]	O
Continental PEC in air (total)	8.11E-15	[mg.m-3]	O
Continental PEC in agricultural soil (total)	7.59E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	4.40E-14	[mg.l-1]	O
Continental PEC in natural soil (total)	8.43E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	8.43E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.16E-10	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	5.78E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	3.07E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	2.92E-15	[mg.l-1]	O
Moderate PEC in air (total)	7.76E-17	[mg.m-3]	O
Moderate PEC in soil (total)	8.08E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	1.21E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	2.77E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	2.63E-15	[mg.l-1]	O
Arctic PEC in air (total)	1.54E-17	[mg.m-3]	O
Arctic PEC in soil (total)	5.06E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	1.10E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.40E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.33E-15	[mg.l-1]	O
Tropic PEC in air (total)	4.80E-17	[mg.m-3]	O
Tropic PEC in soil (total)	2.73E-13	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	5.51E-12	[mg.kgwwt-1]	O

STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.109	[%]	O
Steady-state mass fraction in regional seawater	0.0117	[%]	O
Steady-state mass fraction in regional air	0.0136	[%]	O
Steady-state mass fraction in regional agricultural soil	25.7	[%]	O
Steady-state mass fraction in regional natural soil	3.21	[%]	O
Steady-state mass fraction in regional industrial soil	1.19	[%]	O
Steady-state mass fraction in regional freshwater sediment	4.61	[%]	O
Steady-state mass fraction in regional seawater sediment	0.16	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.46E-03	[%]	O
Steady-state mass fraction in continental seawater	1.5	[%]	O
Steady-state mass fraction in continental air	8.32E-03	[%]	O
Steady-state mass fraction in continental agricultural soil	7.95	[%]	O
Steady-state mass fraction in continental natural soil	0.994	[%]	O
Steady-state mass fraction in continental industrial soil	0.368	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.0614	[%]	O
Steady-state mass fraction in continental seawater sediment	1.02	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	17.5	[%]	O
Steady-state mass fraction in moderate air	8.88E-04	[%]	O
Steady-state mass fraction in moderate soil	0.393	[%]	O
Steady-state mass fraction in moderate sediment	2.4	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	10.4	[%]	O
Steady-state mass fraction in arctic air	9.58E-05	[%]	O
Steady-state mass fraction in arctic soil	0.107	[%]	O
Steady-state mass fraction in arctic sediment	1.42	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	18.3	[%]	O
Steady-state mass fraction in tropic air	8.97E-04	[%]	O
Steady-state mass fraction in tropic soil	0.13	[%]	O
Steady-state mass fraction in tropic sediment	2.49	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	7.45E-04	[kg]	O
Steady-state mass in regional seawater	7.98E-05	[kg]	O

Steady-state mass in regional air	9.25E-05	[kg]	O
Steady-state mass in regional agricultural soil	0.175	[kg]	O
Steady-state mass in regional natural soil	0.0219	[kg]	O
Steady-state mass in regional industrial soil	8.10E-03	[kg]	O
Steady-state mass in regional freshwater sediment	0.0314	[kg]	O
Steady-state mass in regional seawater sediment	1.09E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	9.92E-06	[kg]	O
Steady-state mass in continental seawater	0.0102	[kg]	O
Steady-state mass in continental air	5.67E-05	[kg]	O
Steady-state mass in continental agricultural soil	0.0542	[kg]	O
Steady-state mass in continental natural soil	6.78E-03	[kg]	O
Steady-state mass in continental industrial soil	2.51E-03	[kg]	O
Steady-state mass in continental freshwater sediment	4.19E-04	[kg]	O
Steady-state mass in continental seawater sediment	6.98E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.12	[kg]	O
Steady-state mass in moderate air	6.05E-06	[kg]	O
Steady-state mass in moderate soil	2.68E-03	[kg]	O
Steady-state mass in moderate sediment	0.0163	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0706	[kg]	O
Steady-state mass in arctic air	6.53E-07	[kg]	O
Steady-state mass in arctic soil	7.32E-04	[kg]	O
Steady-state mass in arctic sediment	9.65E-03	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.125	[kg]	O
Steady-state mass in tropic air	6.12E-06	[kg]	O
Steady-state mass in tropic soil	8.89E-04	[kg]	O
Steady-state mass in tropic sediment	0.017	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	8.90E-08	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.15E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	1.15E-07	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.12E-03	[mg.kgdwt-1]	O

Local PEC in seawater during emission episode (dissolved)	1.14E-06	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.14E-06	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.0112	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	2.32E-06	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	2.36E-06	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	4.63E-06	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.21E-09	[mg.l-1]	O
Local PEC in pore water of grassland	2.37E-09	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.21E-09	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D

LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D

Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D
MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S

BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.1	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.01	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.1	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	10	[-]	S
PNEC for marine organisms	0.01	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (fresh)	9.6	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	10	[-]	S
PNEC for fresh-water sediment organisms (from toxicological data)	0.96	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	0.0977	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	No		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	1.92	[mg.kgdwt-1]	O

PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.96	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	9.6	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	10	[-]	S
PNEC for marine sediment organisms (from toxicological data)	0.96	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.0212	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	No		S
PNEC for marine sediment, normalised to 10% o.c. (local)	1.92	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.96	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	15	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	10	[-]	S
PNEC for terrestrial organisms (from toxicological data)	1.5	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.0195	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	No		S
PNEC for terrestrial organisms	1.5	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	0.0115	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.114	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O

RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	5.84E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	5.83E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	1.55E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	1.80E-05	[-]	O
RCR for the regional marine compartment	1.90E-06	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	3.64E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	3.78E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	1.62E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

20.4 Pyrene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Pyrene		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	E6B320A4		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Pyrene		S
Description			D
CAS-No	129-00-0		S
EC-notification no.			D
EINECS no.	204-927-3		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	202.25	[g.mol-1]	S
Melting point	156	[oC]	S
Boiling point	360	[oC]	S
Vapour pressure at test temperature	1.20E-03	[Pa]	S
Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	1.00E-03	[Pa]	S
Octanol-water partition coefficient	4.98	[log10]	S
Water solubility at test temperature	125	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	125	[ug.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	5.89E+04	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	1.4	[Pa.m3.mol-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	1.20E+03	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	1.47E+03	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	5.00E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S

Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	2.24E-05	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	1.10E-04	[ug.m-3]	O
Regional PEC in seawater (total)	1.06E-11	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.01E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	1.03E-11	[mg.l-1]	O

Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.16E-12	[mg.m-3]	O
Regional PEC in agricultural soil (total)	4.88E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	4.70E-12	[mg.l-1]	O
Regional PEC in natural soil (total)	5.32E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	5.32E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	2.56E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	2.54E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.26E-14	[mg.l-1]	O
Continental PEC in seawater (total)	7.03E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.16E-14	[mg.l-1]	O
Continental PEC in seawater (dissolved)	6.82E-15	[mg.l-1]	O
Continental PEC in air (total)	4.14E-15	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.75E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.68E-14	[mg.l-1]	O
Continental PEC in natural soil (total)	1.90E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.90E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.94E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	1.69E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.30E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.26E-15	[mg.l-1]	O
Moderate PEC in air (total)	4.13E-17	[mg.m-3]	O
Moderate PEC in soil (total)	1.90E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	3.13E-12	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.14E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.10E-15	[mg.l-1]	O
Arctic PEC in air (total)	8.42E-18	[mg.m-3]	O
Arctic PEC in soil (total)	1.23E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	2.73E-12	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	5.23E-16	[mg.l-1]	O
Tropic PEC in water (dissolved)	5.07E-16	[mg.l-1]	O
Tropic PEC in air (total)	2.25E-17	[mg.m-3]	O
Tropic PEC in soil (total)	5.68E-14	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	1.26E-12	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			

REGIONAL			
Steady-state mass fraction in regional freshwater	0.183	[%]	O
Steady-state mass fraction in regional seawater	0.0195	[%]	O
Steady-state mass fraction in regional air	0.0215	[%]	O
Steady-state mass fraction in regional agricultural soil	18.3	[%]	O
Steady-state mass fraction in regional natural soil	2.25	[%]	O
Steady-state mass fraction in regional industrial soil	0.832	[%]	O
Steady-state mass fraction in regional freshwater sediment	4.88	[%]	O
Steady-state mass fraction in regional seawater sediment	0.162	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.83E-03	[%]	O
Steady-state mass fraction in continental seawater	2.26	[%]	O
Steady-state mass fraction in continental air	0.0133	[%]	O
Steady-state mass fraction in continental agricultural soil	5.74	[%]	O
Steady-state mass fraction in continental natural soil	0.703	[%]	O
Steady-state mass fraction in continental industrial soil	0.26	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.049	[%]	O
Steady-state mass fraction in continental seawater sediment	0.94	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	23.3	[%]	O
Steady-state mass fraction in moderate air	1.48E-03	[%]	O
Steady-state mass fraction in moderate soil	0.289	[%]	O
Steady-state mass fraction in moderate sediment	1.93	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	13.3	[%]	O
Steady-state mass fraction in arctic air	1.65E-04	[%]	O
Steady-state mass fraction in arctic soil	0.082	[%]	O
Steady-state mass fraction in arctic sediment	1.11	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	21.5	[%]	O
Steady-state mass fraction in tropic air	1.32E-03	[%]	O
Steady-state mass fraction in tropic soil	0.085	[%]	O
Steady-state mass fraction in tropic sediment	1.78	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	3.97E-04	[kg]	O
Steady-state mass in regional seawater	4.23E-05	[kg]	O
Steady-state mass in regional air	4.68E-05	[kg]	O

Steady-state mass in regional agricultural soil	0.0398	[kg]	O
Steady-state mass in regional natural soil	4.88E-03	[kg]	O
Steady-state mass in regional industrial soil	1.81E-03	[kg]	O
Steady-state mass in regional freshwater sediment	0.0106	[kg]	O
Steady-state mass in regional seawater sediment	3.51E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	3.98E-06	[kg]	O
Steady-state mass in continental seawater	4.92E-03	[kg]	O
Steady-state mass in continental air	2.90E-05	[kg]	O
Steady-state mass in continental agricultural soil	0.0125	[kg]	O
Steady-state mass in continental natural soil	1.53E-03	[kg]	O
Steady-state mass in continental industrial soil	5.66E-04	[kg]	O
Steady-state mass in continental freshwater sediment	1.06E-04	[kg]	O
Steady-state mass in continental seawater sediment	2.04E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0507	[kg]	O
Steady-state mass in moderate air	3.22E-06	[kg]	O
Steady-state mass in moderate soil	6.29E-04	[kg]	O
Steady-state mass in moderate sediment	4.21E-03	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0289	[kg]	O
Steady-state mass in arctic air	3.58E-07	[kg]	O
Steady-state mass in arctic soil	1.78E-04	[kg]	O
Steady-state mass in arctic sediment	2.40E-03	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0467	[kg]	O
Steady-state mass in tropic air	2.87E-06	[kg]	O
Steady-state mass in tropic soil	1.85E-04	[kg]	O
Steady-state mass in tropic sediment	3.87E-03	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	4.41E-08	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	6.82E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	6.82E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	4.02E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	6.81E-07	[mg.l-1]	O

Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	6.81E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	4.02E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	9.12E-07	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	9.30E-07	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.82E-06	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	7.90E-10	[mg.l-1]	O
Local PEC in pore water of grassland	1.55E-09	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	7.90E-10	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D

Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D

NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D
MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O

NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S

BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.23	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.023	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.23	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	10	[-]	S
PNEC for marine organisms	0.023	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (fresh)	140	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	50	[-]	S
PNEC for fresh-water sediment organisms (from toxicological data)	2.8	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	0.136	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	No		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	5.6	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	2.8	[mg.kgdwt-1]	O

MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	140	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	100	[-]	S
PNEC for marine sediment organisms (from toxicological data)	1.4	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.0295	[mg.kgwwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	No		S
PNEC for marine sediment, normalised to 10% o.c. (local)	2.8	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	1.4	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	10	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	10	[-]	S
PNEC for terrestrial organisms (from toxicological data)	1	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.0271	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	No		S
PNEC for terrestrial organisms	1	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	2.97E-03	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.0296	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O

SEDIMENT			
RCR for the local fresh-water sediment compartment	7.18E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	1.43E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	9.12E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	4.40E-06	[-]	O
RCR for the regional marine compartment	4.46E-07	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	4.21E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	8.36E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	5.53E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

20.5 Benz[a]anthracene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Benzaant lowfood		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	35A96538		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
CHARACTERISTICS OF HUMANS			
Daily intake of fish	0.024	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.493	[kg.d-1]	S
Daily intake of root crops	0.067	[kg.d-1]	S
Daily intake of meat	0.15	[kg.d-1]	S
Daily intake of dairy products	0.187	[kg.d-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Benzaanthracene		S
Description			D
CAS-No	56-55-3		S
EC-notification no.			D
EINECS no.	200-280-6		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	228.29	[g.mol-1]	S
Melting point	160.7	[oC]	S
Boiling point	435	[oC]	S
Vapour pressure at test temperature	7.60E-06	[Pa]	S

Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	7.60E-06	[Pa]	S
Octanol-water partition coefficient	5.91	[log10]	S
Water solubility at test temperature	10.2	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	10.2	[ug.l-1]	O
PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	5.01E+05	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	0.81	[Pa.m3.mol-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	9.80E+03	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	260	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	1.22E-10	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			

High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	8.79E-06	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			

PECS			
REGIONAL			
Regional PEC in surface water (total)	3.91E-05	[ug.m-3]	O
Regional PEC in seawater (total)	3.72E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	2.23E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	2.97E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.35E-15	[mg.m-3]	O
Regional PEC in agricultural soil (total)	3.84E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	4.35E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	5.91E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	5.91E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	4.86E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	6.44E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	8.67E-17	[mg.l-1]	O
Continental PEC in seawater (total)	3.11E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	4.95E-17	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.49E-15	[mg.l-1]	O
Continental PEC in air (total)	4.44E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.26E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.43E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	1.94E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.94E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.08E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	5.40E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.51E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.21E-15	[mg.l-1]	O
Moderate PEC in air (total)	1.22E-18	[mg.m-3]	O
Moderate PEC in soil (total)	5.33E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	2.62E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.49E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.19E-15	[mg.l-1]	O
Arctic PEC in air (total)	3.95E-19	[mg.m-3]	O
Arctic PEC in soil (total)	2.81E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	2.58E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			

Tropic PEC in water (total)	1.22E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	9.77E-16	[mg.l-1]	O
Tropic PEC in air (total)	2.58E-18	[mg.m-3]	O
Tropic PEC in soil (total)	7.60E-13	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	2.11E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0382	[%]	O
Steady-state mass fraction in regional seawater	4.04E-03	[%]	O
Steady-state mass fraction in regional air	1.48E-05	[%]	O
Steady-state mass fraction in regional agricultural soil	0.851	[%]	O
Steady-state mass fraction in regional natural soil	0.147	[%]	O
Steady-state mass fraction in regional industrial soil	0.0545	[%]	O
Steady-state mass fraction in regional freshwater sediment	5.46	[%]	O
Steady-state mass fraction in regional seawater sediment	0.241	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	7.41E-06	[%]	O
Steady-state mass fraction in continental seawater	0.592	[%]	O
Steady-state mass fraction in continental air	8.43E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.245	[%]	O
Steady-state mass fraction in continental natural soil	0.0423	[%]	O
Steady-state mass fraction in continental industrial soil	0.0157	[%]	O
Steady-state mass fraction in continental freshwater sediment	1.06E-03	[%]	O
Steady-state mass fraction in continental seawater sediment	1.77	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	16	[%]	O
Steady-state mass fraction in moderate air	2.58E-05	[%]	O
Steady-state mass fraction in moderate soil	0.479	[%]	O
Steady-state mass fraction in moderate sediment	9.56	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	10.3	[%]	O
Steady-state mass fraction in arctic air	4.56E-06	[%]	O
Steady-state mass fraction in arctic soil	0.11	[%]	O
Steady-state mass fraction in arctic sediment	6.16	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	29.6	[%]	O
Steady-state mass fraction in tropic air	8.93E-05	[%]	O
Steady-state mass fraction in tropic soil	0.671	[%]	O

Steady-state mass fraction in tropic sediment	17.7	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	1.41E-04	[kg]	O
Steady-state mass in regional seawater	1.49E-05	[kg]	O
Steady-state mass in regional air	5.45E-08	[kg]	O
Steady-state mass in regional agricultural soil	3.14E-03	[kg]	O
Steady-state mass in regional natural soil	5.42E-04	[kg]	O
Steady-state mass in regional industrial soil	2.01E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0201	[kg]	O
Steady-state mass in regional seawater sediment	8.89E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	2.73E-08	[kg]	O
Steady-state mass in continental seawater	2.18E-03	[kg]	O
Steady-state mass in continental air	3.11E-08	[kg]	O
Steady-state mass in continental agricultural soil	9.02E-04	[kg]	O
Steady-state mass in continental natural soil	1.56E-04	[kg]	O
Steady-state mass in continental industrial soil	5.78E-05	[kg]	O
Steady-state mass in continental freshwater sediment	3.90E-06	[kg]	O
Steady-state mass in continental seawater sediment	6.52E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0589	[kg]	O
Steady-state mass in moderate air	9.50E-08	[kg]	O
Steady-state mass in moderate soil	1.77E-03	[kg]	O
Steady-state mass in moderate sediment	0.0352	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.038	[kg]	O
Steady-state mass in arctic air	1.68E-08	[kg]	O
Steady-state mass in arctic soil	4.07E-04	[kg]	O
Steady-state mass in arctic sediment	0.0227	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.109	[kg]	O
Steady-state mass in tropic air	3.29E-07	[kg]	O
Steady-state mass in tropic soil	2.47E-03	[kg]	O
Steady-state mass in tropic sediment	0.0651	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	1.86E-11	[mg.m-3]	O

WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.66E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	1.66E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	8.33E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.66E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.66E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	8.31E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	4.80E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	4.88E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	9.05E-09	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	4.87E-13	[mg.l-1]	O
Local PEC in pore water of grassland	9.03E-13	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	4.87E-13	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D

NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			

EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D

MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D

MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D

CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D

Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S
BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
HUMANS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (repdose)	??	[mg.cm-3]	D
Dermal LOEC in a medium (repdose)	??	[mg.cm-3]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D

Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (fert)	??	[mg.cm-3]	D
Dermal LOEC in a medium (fert)	??	[mg.cm-3]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (mattox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (mattox)	??	[mg.cm-3]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (devtox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (devtox)	??	[mg.cm-3]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
DERMAL			

Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (carc)	??	[mg.cm-3]	D
Dermal LOEC in a medium (carc)	??	[mg.cm-3]	D
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	No		D
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	1.2	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	100	[-]	S
PNEC for aquatic organisms	0.012	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	1.2	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	1000	[-]	S
PNEC for marine organisms	1.20E-03	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC	1.2	[mg.kgdwt-1]	S

sediment (fresh)			
Assessment factor applied in extrapolation to PNEC sediment (fresh)	??	[-]	O
PNEC for fresh-water sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	0.601	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	0.601	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.601	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	1.2	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	??	[-]	O
PNEC for marine sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.0601	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	Yes		S
PNEC for marine sediment, normalised to 10% o.c. (local)	0.0601	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.0601	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	0.79	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	10	[-]	S
PNEC for terrestrial organisms (from toxicological data)	0.079	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.12	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	No		S
PNEC for terrestrial organisms	0.079	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
REFERENCE MOS			

HUMANS EXPOSED TO OR VIA THE ENVIRONMENT			
REPEATED DOSE			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (repdose)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (repdose)	1	[-]	O
FERTILITY			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (fert)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (fert)	1	[-]	O
MATERNAL-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D

Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (mattox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (mattox)	1	[-]	O
DEVELOPMENT-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (devtox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (devtox)	1	[-]	O
CARC (THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (carc)	1	[-]	O

INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (carc)	1	[-]	O
CARC (NON-THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, oral (non-threshold)	2.50E+05	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, inhalatory (non-threshold)	2.50E+05	[-]	O
HUMAN EQUIV. DOSE			
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, inhalatory, non-threshold	1	[-]	O
Human equivalent dose humans via environment, inhalatory, non-threshold	??	[mg.m-3]	O
TOTAL EXPOSURE			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, total, non-threshold	1	[-]	O
Human equivalent dose humans via environment, total, non-threshold	??	[mg.kg-1.d-1]	O
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			

WATER			
RCR for the local fresh-water compartment	1.38E-03	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.138	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	0.0138	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	1.38	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	6.08E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	1.86E-06	[-]	O
RCR for the regional marine compartment	2.48E-06	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	3.72E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	4.93E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	5.52E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O
HUMANS EXPOSED TO OR VIA THE ENVIRONMENTAL			

LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
REPEATED DOSE			
INHALATORY			
MOS, local, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, local, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, local, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	??	[-]	O
DEVELOPMENT-TOX			
INHALATORY			
MOS, local, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, local, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			

MOS, local, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, local, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, local, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, local, exposure via air	??	[-]	O
Lifetime cancer risk, local, total exposure	??	[-]	O
REGIONAL			
REPEATED DOSE			
INHALATORY			
MOS, regional, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, regional, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, regional, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	??	[-]	O

DEVELOPMENT-TOX			
INHALATORY			
MOS, regional, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, regional, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, regional, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, regional, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, regional, exposure via air	??	[-]	O
Lifetime cancer risk, regional, total exposure	??	[-]	O

20.6 Chrysene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Chrysene lowfood		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	4A384684		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
CHARACTERISTICS OF HUMANS			
Daily intake of fish	0.024	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.493	[kg.d-1]	S
Daily intake of root crops	0.067	[kg.d-1]	S
Daily intake of meat	0.15	[kg.d-1]	S
Daily intake of dairy products	0.187	[kg.d-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Chrysene		S
Description			D
CAS-No	218-01-9		S
EC-notification no.			D
EINECS no.	205-923-4		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	228.29	[g.mol-1]	S
Melting point	253.8	[oC]	S
Boiling point	448	[oC]	S
Vapour pressure at test temperature	5.70E-07	[Pa]	S

Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	5.70E-07	[Pa]	S
Octanol-water partition coefficient	5.81	[log10]	S
Water solubility at test temperature	1.65	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	1.65	[ug.l-1]	O
PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	3.98E+05	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	0.079	[Pa.m3.mol-1]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	7.80E+03	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	6.09E+03	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	8.00E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			

High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	1.13E-05	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			

PECS			
REGIONAL			
Regional PEC in surface water (total)	5.56E-05	[ug.m-3]	O
Regional PEC in seawater (total)	5.31E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	3.47E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	4.41E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.40E-15	[mg.m-3]	O
Regional PEC in agricultural soil (total)	5.25E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	7.48E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	8.52E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	8.52E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	5.99E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	7.59E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.95E-16	[mg.l-1]	O
Continental PEC in seawater (total)	5.80E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.22E-16	[mg.l-1]	O
Continental PEC in seawater (dissolved)	4.82E-15	[mg.l-1]	O
Continental PEC in air (total)	6.23E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	2.34E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	3.33E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	3.79E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.79E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.10E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	8.29E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	3.50E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	2.90E-15	[mg.l-1]	O
Moderate PEC in air (total)	2.02E-18	[mg.m-3]	O
Moderate PEC in soil (total)	1.23E-12	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	4.99E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	3.47E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	2.88E-15	[mg.l-1]	O
Arctic PEC in air (total)	6.65E-19	[mg.m-3]	O
Arctic PEC in soil (total)	5.84E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	4.95E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			

Tropic PEC in water (total)	3.06E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	2.54E-15	[mg.l-1]	O
Tropic PEC in air (total)	4.58E-18	[mg.m-3]	O
Tropic PEC in soil (total)	2.02E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	4.36E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0249	[%]	O
Steady-state mass fraction in regional seawater	2.65E-03	[%]	O
Steady-state mass fraction in regional air	7.06E-06	[%]	O
Steady-state mass fraction in regional agricultural soil	0.534	[%]	O
Steady-state mass fraction in regional natural soil	0.0975	[%]	O
Steady-state mass fraction in regional industrial soil	0.0361	[%]	O
Steady-state mass fraction in regional freshwater sediment	3.09	[%]	O
Steady-state mass fraction in regional seawater sediment	0.131	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	7.65E-06	[%]	O
Steady-state mass fraction in continental seawater	0.506	[%]	O
Steady-state mass fraction in continental air	5.44E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.208	[%]	O
Steady-state mass fraction in continental natural soil	0.0379	[%]	O
Steady-state mass fraction in continental industrial soil	0.0141	[%]	O
Steady-state mass fraction in continental freshwater sediment	9.48E-04	[%]	O
Steady-state mass fraction in continental seawater sediment	1.25	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	17	[%]	O
Steady-state mass fraction in moderate air	1.96E-05	[%]	O
Steady-state mass fraction in moderate soil	0.507	[%]	O
Steady-state mass fraction in moderate sediment	8.37	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	11	[%]	O
Steady-state mass fraction in arctic air	3.52E-06	[%]	O
Steady-state mass fraction in arctic soil	0.105	[%]	O
Steady-state mass fraction in arctic sediment	5.43	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	34.1	[%]	O
Steady-state mass fraction in tropic air	7.29E-05	[%]	O
Steady-state mass fraction in tropic soil	0.817	[%]	O

Steady-state mass fraction in tropic sediment	16.8	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	2.00E-04	[kg]	O
Steady-state mass in regional seawater	2.13E-05	[kg]	O
Steady-state mass in regional air	5.66E-08	[kg]	O
Steady-state mass in regional agricultural soil	4.29E-03	[kg]	O
Steady-state mass in regional natural soil	7.82E-04	[kg]	O
Steady-state mass in regional industrial soil	2.90E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0248	[kg]	O
Steady-state mass in regional seawater sediment	1.05E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	6.14E-08	[kg]	O
Steady-state mass in continental seawater	4.06E-03	[kg]	O
Steady-state mass in continental air	4.36E-08	[kg]	O
Steady-state mass in continental agricultural soil	1.67E-03	[kg]	O
Steady-state mass in continental natural soil	3.04E-04	[kg]	O
Steady-state mass in continental industrial soil	1.13E-04	[kg]	O
Steady-state mass in continental freshwater sediment	7.61E-06	[kg]	O
Steady-state mass in continental seawater sediment	0.01	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.136	[kg]	O
Steady-state mass in moderate air	1.57E-07	[kg]	O
Steady-state mass in moderate soil	4.07E-03	[kg]	O
Steady-state mass in moderate sediment	0.0671	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0884	[kg]	O
Steady-state mass in arctic air	2.82E-08	[kg]	O
Steady-state mass in arctic soil	8.44E-04	[kg]	O
Steady-state mass in arctic sediment	0.0436	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.273	[kg]	O
Steady-state mass in tropic air	5.85E-07	[kg]	O
Steady-state mass in tropic soil	6.56E-03	[kg]	O
Steady-state mass in tropic sediment	0.134	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	1.86E-11	[mg.m-3]	O

WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	2.35E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	2.35E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	9.35E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	2.35E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	2.35E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	9.34E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	5.84E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	5.94E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.09E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	7.46E-13	[mg.l-1]	O
Local PEC in pore water of grassland	1.37E-12	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	7.46E-13	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D

NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			

EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D

MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D

MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D

CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D

Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S
BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
HUMANS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (repdose)	??	[mg.cm-3]	D
Dermal LOEC in a medium (repdose)	??	[mg.cm-3]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D

Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (fert)	??	[mg.cm-3]	D
Dermal LOEC in a medium (fert)	??	[mg.cm-3]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (mattox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (mattox)	??	[mg.cm-3]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (devtox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (devtox)	??	[mg.cm-3]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
DERMAL			

Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (carc)	??	[mg.cm-3]	D
Dermal LOEC in a medium (carc)	??	[mg.cm-3]	D
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	No		D
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.7	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.07	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.7	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	100	[-]	S
PNEC for marine organisms	7.00E-03	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC	0.7	[mg.kgdwt-1]	S

sediment (fresh)			
Assessment factor applied in extrapolation to PNEC sediment (fresh)	??	[-]	O
PNEC for fresh-water sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	2.79	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	2.79	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	2.79	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	0.7	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	??	[-]	O
PNEC for marine sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.279	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	Yes		S
PNEC for marine sediment, normalised to 10% o.c. (local)	0.279	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.279	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	0.7	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	??	[-]	O
PNEC for terrestrial organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.557	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		S
PNEC for terrestrial organisms	0.557	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
REFERENCE MOS			

HUMANS EXPOSED TO OR VIA THE ENVIRONMENT			
REPEATED DOSE			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (repdose)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (repdose)	1	[-]	O
FERTILITY			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (fert)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (fert)	1	[-]	O
MATERNAL-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D

Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (mattox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (mattox)	1	[-]	O
DEVELOPMENT-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (devtox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (devtox)	1	[-]	O
CARC (THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (carc)	1	[-]	O

INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (carc)	1	[-]	O
CARC (NON-THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, oral (non-threshold)	2.50E+05	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, inhalatory (non-threshold)	2.50E+05	[-]	O
HUMAN EQUIV. DOSE			
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, inhalatory, non-threshold	1	[-]	O
Human equivalent dose humans via environment, inhalatory, non-threshold	??	[mg.m-3]	O
TOTAL EXPOSURE			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, total, non-threshold	1	[-]	O
Human equivalent dose humans via environment, total, non-threshold	??	[mg.kg-1.d-1]	O
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			

WATER			
RCR for the local fresh-water compartment	3.36E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.0335	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	3.36E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	0.335	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.05E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	4.95E-07	[-]	O
RCR for the regional marine compartment	6.30E-07	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	9.88E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	1.25E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	1.07E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional soil compartment, statistical method	??	[-]	O
HUMANS EXPOSED TO OR VIA THE ENVIRONMENTAL			

LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
REPEATED DOSE			
INHALATORY			
MOS, local, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, local, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, local, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	??	[-]	O
DEVELOPMENT-TOX			
INHALATORY			
MOS, local, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, local, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			

MOS, local, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, local, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, local, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, local, exposure via air	??	[-]	O
Lifetime cancer risk, local, total exposure	??	[-]	O
REGIONAL			
REPEATED DOSE			
INHALATORY			
MOS, regional, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, regional, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, regional, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	??	[-]	O

DEVELOPMENT-TOX			
INHALATORY			
MOS, regional, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, regional, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, regional, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, regional, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, regional, exposure via air	??	[-]	O
Lifetime cancer risk, regional, total exposure	??	[-]	O

20.7 Benzo[a]pyrene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Benzoapy lowfood		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	4E90266B		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
CHARACTERISTICS OF HUMANS			
Daily intake of fish	0.024	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.493	[kg.d-1]	S
Daily intake of root crops	0.067	[kg.d-1]	S
Daily intake of meat	0.15	[kg.d-1]	S
Daily intake of dairy products	0.187	[kg.d-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Benzoapyrene		S
Description			D
CAS-No	50-32-8		S
EC-notification no.			D
EINECS no.	200-028-5		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	252.31	[g.mol-1]	S
Melting point	175	[oC]	S
Boiling point	496	[oC]	S
Vapour pressure at test temperature	7.30E-07	[Pa]	S

Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	7.30E-07	[Pa]	O
Octanol-water partition coefficient	6.13	[log10]	S
Water solubility at test temperature	1.54	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	1.54	[ug.l-1]	O
PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	8.32E+05	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	0.034	[Pa.m3.mol-1]	S
Temperature at which Henry's law constant was measured	20	[oC]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	1.60E+04	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	608	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	5.00E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			

CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	8.60E-06	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	3.30E-08	[mg.m-3]	O
Regional PEC in seawater (total)	3.10E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.47E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	2.19E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.30E-15	[mg.m-3]	O
Regional PEC in agricultural soil (total)	6.73E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	4.58E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	1.20E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	1.20E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	5.31E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	7.90E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.91E-16	[mg.l-1]	O
Continental PEC in seawater (total)	3.12E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	8.48E-17	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.20E-15	[mg.l-1]	O
Continental PEC in air (total)	7.29E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.77E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.57E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	6.72E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	6.72E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	3.06E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	7.94E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.77E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.25E-15	[mg.l-1]	O
Moderate PEC in air (total)	1.92E-18	[mg.m-3]	O
Moderate PEC in soil (total)	1.77E-12	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	4.51E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.75E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.24E-15	[mg.l-1]	O
Arctic PEC in air (total)	6.61E-19	[mg.m-3]	O
Arctic PEC in soil (total)	6.59E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	4.47E-11	[mg.kgwwt-1]	O

GLOBAL: TROPIC			
Tropic PEC in water (total)	1.52E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.08E-15	[mg.l-1]	O
Tropic PEC in air (total)	3.98E-18	[mg.m-3]	O
Tropic PEC in soil (total)	3.07E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	3.87E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0224	[%]	O
Steady-state mass fraction in regional seawater	2.34E-03	[%]	O
Steady-state mass fraction in regional air	9.91E-06	[%]	O
Steady-state mass fraction in regional agricultural soil	1.03	[%]	O
Steady-state mass fraction in regional natural soil	0.207	[%]	O
Steady-state mass fraction in regional industrial soil	0.0768	[%]	O
Steady-state mass fraction in regional freshwater sediment	4.14	[%]	O
Steady-state mass fraction in regional seawater sediment	0.205	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.13E-05	[%]	O
Steady-state mass fraction in continental seawater	0.411	[%]	O
Steady-state mass fraction in continental air	9.61E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.507	[%]	O
Steady-state mass fraction in continental natural soil	0.102	[%]	O
Steady-state mass fraction in continental industrial soil	0.0376	[%]	O
Steady-state mass fraction in continental freshwater sediment	2.09E-03	[%]	O
Steady-state mass fraction in continental seawater sediment	1.8	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	13	[%]	O
Steady-state mass fraction in moderate air	2.81E-05	[%]	O
Steady-state mass fraction in moderate soil	1.1	[%]	O
Steady-state mass fraction in moderate sediment	11.4	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	8.42	[%]	O
Steady-state mass fraction in arctic air	5.29E-06	[%]	O
Steady-state mass fraction in arctic soil	0.179	[%]	O
Steady-state mass fraction in arctic sediment	7.4	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	25.6	[%]	O
Steady-state mass fraction in tropic air	9.56E-05	[%]	O

Steady-state mass fraction in tropic soil	1.88	[%]	O
Steady-state mass fraction in tropic sediment	22.4	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	1.19E-04	[kg]	O
Steady-state mass in regional seawater	1.24E-05	[kg]	O
Steady-state mass in regional air	5.26E-08	[kg]	O
Steady-state mass in regional agricultural soil	5.49E-03	[kg]	O
Steady-state mass in regional natural soil	1.10E-03	[kg]	O
Steady-state mass in regional industrial soil	4.08E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.022	[kg]	O
Steady-state mass in regional seawater sediment	1.09E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	6.00E-08	[kg]	O
Steady-state mass in continental seawater	2.18E-03	[kg]	O
Steady-state mass in continental air	5.10E-08	[kg]	O
Steady-state mass in continental agricultural soil	2.69E-03	[kg]	O
Steady-state mass in continental natural soil	5.39E-04	[kg]	O
Steady-state mass in continental industrial soil	2.00E-04	[kg]	O
Steady-state mass in continental freshwater sediment	1.11E-05	[kg]	O
Steady-state mass in continental seawater sediment	9.58E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0691	[kg]	O
Steady-state mass in moderate air	1.49E-07	[kg]	O
Steady-state mass in moderate soil	5.85E-03	[kg]	O
Steady-state mass in moderate sediment	0.0606	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0447	[kg]	O
Steady-state mass in arctic air	2.81E-08	[kg]	O
Steady-state mass in arctic soil	9.52E-04	[kg]	O
Steady-state mass in arctic sediment	0.0393	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.136	[kg]	O
Steady-state mass in tropic air	5.07E-07	[kg]	O
Steady-state mass in tropic soil	9.97E-03	[kg]	O
Steady-state mass in tropic sediment	0.119	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			

Annual average local PEC in air (total)	1.86E-11	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.27E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	1.27E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.05E-03	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.26E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.26E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.0105	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	8.54E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	8.68E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.60E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	5.22E-13	[mg.l-1]	O
Local PEC in pore water of grassland	9.62E-13	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	5.22E-13	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D

NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D

EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D

MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D

Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D

Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D

Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S
BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
HUMANS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (repdose)	??	[mg.cm-3]	D
Dermal LOEC in a medium (repdose)	??	[mg.cm-3]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
DERMAL			

Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (fert)	??	[mg.cm-3]	D
Dermal LOEC in a medium (fert)	??	[mg.cm-3]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (mattox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (mattox)	??	[mg.cm-3]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (devtox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (devtox)	??	[mg.cm-3]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D

DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (carc)	??	[mg.cm-3]	D
Dermal LOEC in a medium (carc)	??	[mg.cm-3]	D
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	No		D
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.22	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.022	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.22	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	10	[-]	S
PNEC for marine organisms	0.022	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			

Toxicological data used for extrapolation to PNEC sediment (fresh)	0.22	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	??	[-]	O
PNEC for fresh-water sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	1.83	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	1.83	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	1.83	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	0.22	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	??	[-]	O
PNEC for marine sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	1.83	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	Yes		S
PNEC for marine sediment, normalised to 10% o.c. (local)	1.83	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	1.83	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	0.53	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	10	[-]	S
PNEC for terrestrial organisms (from toxicological data)	0.053	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.366	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	No		S
PNEC for terrestrial organisms	0.053	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			

REFERENCE MOS			
HUMANS EXPOSED TO OR VIA THE ENVIRONMENT			
REPEATED DOSE			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (repdose)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (repdose)	1	[-]	O
FERTILITY			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (fert)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (fert)	1	[-]	O
MATERNAL-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D

Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (mattox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (mattox)	1	[-]	O
DEVELOPMENT-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (devtox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (devtox)	1	[-]	O
CARC (THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (carc)	1	[-]	O

INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (carc)	1	[-]	O
CARC (NON-THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, oral (non-threshold)	2.50E+05	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, inhalatory (non-threshold)	2.50E+05	[-]	O
HUMAN EQUIV. DOSE			
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, inhalatory, non-threshold	1	[-]	O
Human equivalent dose humans via environment, inhalatory, non-threshold	??	[mg.m-3]	O
TOTAL EXPOSURE			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, total, non-threshold	1	[-]	O
Human equivalent dose humans via environment, total, non-threshold	??	[mg.kg-1.d-1]	O
ENVIRONMENTAL EXPOSURE			
LOCAL			

RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	5.75E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	5.75E-03	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	5.75E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	0.0575	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.61E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		S
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	6.68E-07	[-]	O
RCR for the regional marine compartment	9.96E-08	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	1.33E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	1.99E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	1.44E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

HUMANS EXPOSED TO OR VIA THE ENVIRONMENTAL			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
REPEATED DOSE			
INHALATORY			
MOS, local, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, local, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, local, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	??	[-]	O
DEVELOPMENT-TOX			
INHALATORY			
MOS, local, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, local, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (carc)	??	[-]	O

TOTAL EXPOSURE			
MOS, local, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, local, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, local, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, local, exposure via air	??	[-]	O
Lifetime cancer risk, local, total exposure	??	[-]	O
REGIONAL			
REPEATED DOSE			
INHALATORY			
MOS, regional, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, regional, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, regional, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	??	[-]	O

DEVELOPMENT-TOX			
INHALATORY			
MOS, regional, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, regional, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, regional, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, regional, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, regional, exposure via air	??	[-]	O
Lifetime cancer risk, regional, total exposure	??	[-]	O

20.8 Benzo[b]fluoranthene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Benzobfl lowfood		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	330972F9		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
CHARACTERISTICS OF HUMANS			
Daily intake of fish	0.024	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.493	[kg.d-1]	S
Daily intake of root crops	0.067	[kg.d-1]	S
Daily intake of meat	0.15	[kg.d-1]	S
Daily intake of dairy products	0.187	[kg.d-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Benzobfluoranthene		S
Description			D
CAS-No	205-99-2		S
EC-notification no.			D
EINECS no.	205-911-9		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	252.31	[g.mol-1]	S
Melting point	168.3	[oC]	S
Boiling point	481	[oC]	S
Vapour pressure at test temperature	3.30E-06	[Pa]	S

Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	3.30E-06	[Pa]	O
Octanol-water partition coefficient	6.12	[log10]	S
Water solubility at test temperature	1.28	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	1.28	[ug.l-1]	O
PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	8.32E+05	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	0.051	[Pa.m3.mol-1]	S
Temperature at which Henry's law constant was measured	20	[oC]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	1.60E+04	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	1.86E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			

High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			
Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	1.55E-05	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			

PECS			
REGIONAL			
Regional PEC in surface water (total)	5.67E-05	[ug.m-3]	O
Regional PEC in seawater (total)	5.30E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	2.48E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	3.65E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.29E-14	[mg.m-3]	O
Regional PEC in agricultural soil (total)	3.26E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	2.22E-13	[mg.l-1]	O
Regional PEC in natural soil (total)	4.50E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	4.50E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	8.97E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	1.31E-07	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.53E-15	[mg.l-1]	O
Continental PEC in seawater (total)	3.55E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	6.71E-16	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.45E-15	[mg.l-1]	O
Continental PEC in air (total)	1.30E-16	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.28E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.24E-15	[mg.l-1]	O
Continental PEC in natural soil (total)	4.54E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	4.54E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.43E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	8.82E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.27E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	8.76E-16	[mg.l-1]	O
Moderate PEC in air (total)	1.67E-17	[mg.m-3]	O
Moderate PEC in soil (total)	5.83E-12	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	3.16E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.23E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	8.44E-16	[mg.l-1]	O
Arctic PEC in air (total)	6.03E-18	[mg.m-3]	O
Arctic PEC in soil (total)	3.22E-12	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	3.04E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			

Tropic PEC in water (total)	8.94E-16	[mg.l-1]	O
Tropic PEC in water (dissolved)	6.16E-16	[mg.l-1]	O
Tropic PEC in air (total)	2.39E-17	[mg.m-3]	O
Tropic PEC in soil (total)	6.27E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	2.22E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0448	[%]	O
Steady-state mass fraction in regional seawater	4.65E-03	[%]	O
Steady-state mass fraction in regional air	1.15E-04	[%]	O
Steady-state mass fraction in regional agricultural soil	5.84	[%]	O
Steady-state mass fraction in regional natural soil	0.907	[%]	O
Steady-state mass fraction in regional industrial soil	0.336	[%]	O
Steady-state mass fraction in regional freshwater sediment	8.15	[%]	O
Steady-state mass fraction in regional seawater sediment	0.398	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.06E-04	[%]	O
Steady-state mass fraction in continental seawater	0.546	[%]	O
Steady-state mass fraction in continental air	2.00E-04	[%]	O
Steady-state mass fraction in continental agricultural soil	5.15	[%]	O
Steady-state mass fraction in continental natural soil	0.8	[%]	O
Steady-state mass fraction in continental industrial soil	0.296	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.0193	[%]	O
Steady-state mass fraction in continental seawater sediment	2.34	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	10.9	[%]	O
Steady-state mass fraction in moderate air	2.87E-04	[%]	O
Steady-state mass fraction in moderate soil	4.24	[%]	O
Steady-state mass fraction in moderate sediment	9.32	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	6.86	[%]	O
Steady-state mass fraction in arctic air	5.63E-05	[%]	O
Steady-state mass fraction in arctic soil	1.02	[%]	O
Steady-state mass fraction in arctic sediment	5.88	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	17.5	[%]	O
Steady-state mass fraction in tropic air	6.70E-04	[%]	O
Steady-state mass fraction in tropic soil	4.48	[%]	O

Steady-state mass fraction in tropic sediment	15	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	2.04E-04	[kg]	O
Steady-state mass in regional seawater	2.12E-05	[kg]	O
Steady-state mass in regional air	5.23E-07	[kg]	O
Steady-state mass in regional agricultural soil	0.0266	[kg]	O
Steady-state mass in regional natural soil	4.13E-03	[kg]	O
Steady-state mass in regional industrial soil	1.53E-03	[kg]	O
Steady-state mass in regional freshwater sediment	0.0371	[kg]	O
Steady-state mass in regional seawater sediment	1.81E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	4.83E-07	[kg]	O
Steady-state mass in continental seawater	2.49E-03	[kg]	O
Steady-state mass in continental air	9.13E-07	[kg]	O
Steady-state mass in continental agricultural soil	0.0234	[kg]	O
Steady-state mass in continental natural soil	3.64E-03	[kg]	O
Steady-state mass in continental industrial soil	1.35E-03	[kg]	O
Steady-state mass in continental freshwater sediment	8.78E-05	[kg]	O
Steady-state mass in continental seawater sediment	0.0107	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0496	[kg]	O
Steady-state mass in moderate air	1.31E-06	[kg]	O
Steady-state mass in moderate soil	0.0193	[kg]	O
Steady-state mass in moderate sediment	0.0425	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0312	[kg]	O
Steady-state mass in arctic air	2.56E-07	[kg]	O
Steady-state mass in arctic soil	4.65E-03	[kg]	O
Steady-state mass in arctic sediment	0.0268	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0798	[kg]	O
Steady-state mass in tropic air	3.05E-06	[kg]	O
Steady-state mass in tropic soil	0.0204	[kg]	O
Steady-state mass in tropic sediment	0.0682	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	1.86E-11	[mg.m-3]	O

WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	2.28E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	2.28E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.89E-03	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	2.28E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	2.28E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	0.0189	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.05E-08	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.06E-08	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.61E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	6.37E-13	[mg.l-1]	O
Local PEC in pore water of grassland	9.67E-13	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	6.37E-13	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D

NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			

EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D

MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D

MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D

CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D

Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S
BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
HUMANS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (repdose)	??	[mg.cm-3]	D
Dermal LOEC in a medium (repdose)	??	[mg.cm-3]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D

Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (fert)	??	[mg.cm-3]	D
Dermal LOEC in a medium (fert)	??	[mg.cm-3]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (mattox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (mattox)	??	[mg.cm-3]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (devtox)	??	[mg.cm-3]	D
Dermal LOEC in a medium (devtox)	??	[mg.cm-3]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
DERMAL			

Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal NOEC in a medium (carc)	??	[mg.cm-3]	D
Dermal LOEC in a medium (carc)	??	[mg.cm-3]	D
CURRENT CLASSIFICATION			
Corrosive (C, R34 or R35)	No		D
Irritating to skin (Xi, R38)	No		D
Irritating to eyes (Xi, R36)	No		D
Risk of serious damage to eyes (Xi, R41)	No		D
Irritating to respiratory system (Xi, R37)	No		D
May cause sensitisation by inhalation (Xn, R42)	No		D
May cause sensitisation by skin contact (Xi, R43)	No		D
May cause cancer (T, R45)	No		D
May cause cancer by inhalation (T, R49)	No		D
Possible risk of irreversible effects (Xn, R40)	No		D
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.17	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.017	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.17	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	100	[-]	S
PNEC for marine organisms	1.70E-03	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC	0.17	[mg.kgdwt-1]	S

sediment (fresh)			
Assessment factor applied in extrapolation to PNEC sediment (fresh)	??	[-]	O
PNEC for fresh-water sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	1.41	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	1.41	[mg.kgdwt-1]	O
PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	1.41	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	0.17	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	??	[-]	O
PNEC for marine sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.141	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	Yes		S
PNEC for marine sediment, normalised to 10% o.c. (local)	0.141	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.141	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	0.17	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	??	[-]	O
PNEC for terrestrial organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.283	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		S
PNEC for terrestrial organisms	0.283	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
REFERENCE MOS			

HUMANS EXPOSED TO OR VIA THE ENVIRONMENT			
REPEATED DOSE			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (repdose)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (repdose)	1	[-]	O
FERTILITY			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (fert)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (fert)	1	[-]	O
MATERNAL-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D

Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (mattox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (mattox)	1	[-]	O
DEVELOPMENT-TOX			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (devtox)	1	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (devtox)	1	[-]	O
CARC (THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, oral (carc)	1	[-]	O

INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for intraspecies differences	1	[-]	D
Assessment factor for differences in exposure duration	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Reference-MOS, human environmental, inhalatory (carc)	1	[-]	O
CARC (NON-THRESHOLD)			
ORAL			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, oral (non-threshold)	2.50E+05	[-]	O
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for remaining interspecies differences	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor for dose-response relationship	1	[-]	D
Assessment factor for extrapolation to a low-risk level	2.50E+05	[-]	D
Reference-MOE, human environmental, inhalatory (non-threshold)	2.50E+05	[-]	O
HUMAN EQUIV. DOSE			
INHALATORY			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, inhalatory, non-threshold	1	[-]	O
Human equivalent dose humans via environment, inhalatory, non-threshold	??	[mg.m-3]	O
TOTAL EXPOSURE			
Assessment factor for allometric scaling	1	[-]	D
Assessment factor for differences in exposure route	1	[-]	D
Assessment factor humans via environment, total, non-threshold	1	[-]	O
Human equivalent dose humans via environment, total, non-threshold	??	[mg.kg-1.d-1]	O
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			

WATER			
RCR for the local fresh-water compartment	1.34E-03	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.134	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O
RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	0.0134	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	1.34	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	3.71E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	1.46E-06	[-]	O
RCR for the regional marine compartment	2.15E-06	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	2.92E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	4.28E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	1.31E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional soil compartment, statistical method	??	[-]	O
HUMANS EXPOSED TO OR VIA THE ENVIRONMENTAL			

LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
REPEATED DOSE			
INHALATORY			
MOS, local, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, local, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, local, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (mattox)	??	[-]	O
DEVELOPMENT-TOX			
INHALATORY			
MOS, local, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, local, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, local, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			

MOS, local, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, local, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, local, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, local, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, local, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, local, exposure via air	??	[-]	O
Lifetime cancer risk, local, total exposure	??	[-]	O
REGIONAL			
REPEATED DOSE			
INHALATORY			
MOS, regional, inhalatory (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (repdose)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (repdose)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (repdose)	??	[-]	O
FERTILITY			
INHALATORY			
MOS, regional, inhalatory (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (fert)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (fert)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (fert)	??	[-]	O
MATERNAL-TOX			
INHALATORY			
MOS, regional, inhalatory (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (mattox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (mattox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (mattox)	??	[-]	O

DEVELOPMENT-TOX			
INHALATORY			
MOS, regional, inhalatory (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (devtox)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (devtox)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (devtox)	??	[-]	O
CARC (THRESHOLD)			
INHALATORY			
MOS, regional, inhalatory (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, inhalatory (carc)	??	[-]	O
TOTAL EXPOSURE			
MOS, regional, total exposure (carc)	??	[-]	O
Ratio MOS/Ref-MOS, regional, total exposure (carc)	??	[-]	O
CARC (NON-THRESHOLD)			
INHALATORY			
MOE, regional, inhalatory (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, inhalatory (non-threshold)	??	[-]	O
TOTAL EXPOSURE			
MOE, regional, total exposure (non-threshold)	??	[-]	O
Ratio MOE/Ref-MOE, regional, total exposure (non-threshold)	??	[-]	O
LIFETIME CANCER RISK			
Lifetime cancer risk, regional, exposure via air	??	[-]	O
Lifetime cancer risk, regional, total exposure	??	[-]	O

20.9 Benzozo[k]fluoranthene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Benzokfluorant		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	76E95AF8		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Benzokfluoranthene		S
Description			D
CAS-No	207-08-9		S
EC-notification no.			D
EINECS no.	205-916-6		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	252.31	[g.mol-1]	S
Melting point	217	[oC]	S
Boiling point	480	[oC]	S
Vapour pressure at test temperature	1.30E-07	[Pa]	S
Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	1.30E-07	[Pa]	O
Octanol-water partition coefficient	6.11	[log10]	S
Water solubility at test temperature	0.93	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	0.93	[ug.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	7.94E+05	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	0.043	[Pa.m3.mol-1]	S
Temperature at which Henry's law constant was measured	20	[oC]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	1.50E+04	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	1.32E+04	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	5.36E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			

Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	7.24E-06	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	2.86E-05	[ug.m-3]	O
Regional PEC in seawater (total)	2.70E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.30E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O

Regional PEC in seawater (dissolved)	1.91E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	6.16E-16	[mg.m-3]	O
Regional PEC in agricultural soil (total)	3.84E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	2.74E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	7.58E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	7.58E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	4.48E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	6.58E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	9.78E-17	[mg.l-1]	O
Continental PEC in seawater (total)	3.72E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	4.44E-17	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.64E-15	[mg.l-1]	O
Continental PEC in air (total)	2.86E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.78E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.27E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	3.52E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.52E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.53E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	9.07E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	2.54E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.80E-15	[mg.l-1]	O
Moderate PEC in air (total)	7.61E-19	[mg.m-3]	O
Moderate PEC in soil (total)	9.37E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	6.20E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	2.53E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.79E-15	[mg.l-1]	O
Arctic PEC in air (total)	2.64E-19	[mg.m-3]	O
Arctic PEC in soil (total)	3.08E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	6.18E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	2.32E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.64E-15	[mg.l-1]	O
Tropic PEC in air (total)	1.69E-18	[mg.m-3]	O
Tropic PEC in soil (total)	1.82E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	5.64E-11	[mg.kgwwt-1]	O

STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0141	[%]	O
Steady-state mass fraction in regional seawater	1.48E-03	[%]	O
Steady-state mass fraction in regional air	3.41E-06	[%]	O
Steady-state mass fraction in regional agricultural soil	0.429	[%]	O
Steady-state mass fraction in regional natural soil	0.0953	[%]	O
Steady-state mass fraction in regional industrial soil	0.0353	[%]	O
Steady-state mass fraction in regional freshwater sediment	2.54	[%]	O
Steady-state mass fraction in regional seawater sediment	0.124	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	4.22E-06	[%]	O
Steady-state mass fraction in continental seawater	0.356	[%]	O
Steady-state mass fraction in continental air	2.74E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.174	[%]	O
Steady-state mass fraction in continental natural soil	0.0388	[%]	O
Steady-state mass fraction in continental industrial soil	0.0144	[%]	O
Steady-state mass fraction in continental freshwater sediment	7.59E-04	[%]	O
Steady-state mass fraction in continental seawater sediment	1.5	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	13.6	[%]	O
Steady-state mass fraction in moderate air	8.13E-06	[%]	O
Steady-state mass fraction in moderate soil	0.425	[%]	O
Steady-state mass fraction in moderate sediment	11.4	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	8.83	[%]	O
Steady-state mass fraction in arctic air	1.54E-06	[%]	O
Steady-state mass fraction in arctic soil	0.061	[%]	O
Steady-state mass fraction in arctic sediment	7.44	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	28.3	[%]	O
Steady-state mass fraction in tropic air	2.95E-05	[%]	O
Steady-state mass fraction in tropic soil	0.81	[%]	O
Steady-state mass fraction in tropic sediment	23.8	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	1.03E-04	[kg]	O
Steady-state mass in regional seawater	1.08E-05	[kg]	O

Steady-state mass in regional air	2.49E-08	[kg]	O
Steady-state mass in regional agricultural soil	3.13E-03	[kg]	O
Steady-state mass in regional natural soil	6.96E-04	[kg]	O
Steady-state mass in regional industrial soil	2.58E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0185	[kg]	O
Steady-state mass in regional seawater sediment	9.09E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	3.08E-08	[kg]	O
Steady-state mass in continental seawater	2.60E-03	[kg]	O
Steady-state mass in continental air	2.00E-08	[kg]	O
Steady-state mass in continental agricultural soil	1.27E-03	[kg]	O
Steady-state mass in continental natural soil	2.83E-04	[kg]	O
Steady-state mass in continental industrial soil	1.05E-04	[kg]	O
Steady-state mass in continental freshwater sediment	5.54E-06	[kg]	O
Steady-state mass in continental seawater sediment	0.011	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0991	[kg]	O
Steady-state mass in moderate air	5.94E-08	[kg]	O
Steady-state mass in moderate soil	3.11E-03	[kg]	O
Steady-state mass in moderate sediment	0.0834	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0645	[kg]	O
Steady-state mass in arctic air	1.12E-08	[kg]	O
Steady-state mass in arctic soil	4.45E-04	[kg]	O
Steady-state mass in arctic sediment	0.0543	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.207	[kg]	O
Steady-state mass in tropic air	2.16E-07	[kg]	O
Steady-state mass in tropic soil	5.91E-03	[kg]	O
Steady-state mass in tropic sediment	0.174	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	1.86E-11	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.09E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	1.09E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	8.69E-04	[mg.kgdwt-1]	O

Local PEC in seawater during emission episode (dissolved)	1.09E-07	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.09E-07	[mg.l-1]	O
Local PEC in marine sediment during emission episode	8.68E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	8.52E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	8.68E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.65E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	5.47E-13	[mg.l-1]	O
Local PEC in pore water of grassland	1.04E-12	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	5.47E-13	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D

LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D

Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D
MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S

BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.17	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	0.017	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.17	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	100	[-]	S
PNEC for marine organisms	1.70E-03	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (fresh)	0.17	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	??	[-]	O
PNEC for fresh-water sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	1.35	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	1.35	[mg.kgdwt-1]	O

PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	1.35	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	0.17	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	??	[-]	O
PNEC for marine sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.135	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	Yes		S
PNEC for marine sediment, normalised to 10% o.c. (local)	0.135	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.135	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	0.17	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	??	[-]	O
PNEC for terrestrial organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.27	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		S
PNEC for terrestrial organisms	0.27	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	6.44E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.0643	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O

RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	6.44E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	0.643	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	3.16E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	7.64E-07	[-]	O
RCR for the regional marine compartment	1.13E-06	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	1.53E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	2.24E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	1.61E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional soil compartment, statistical method	??	[-]	O

20.10 Benzo[ghi]perylene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA RainCarbon Benzoghiper		S
Study description	Environment		S
Author			S
Institute			D
Address			D
Zip code			D
City			D
Country			D
Telephone			D
Telefax			D
Email			D
Calculations checksum	F9F17653		S
DEFAULTS			
LOCAL DISTRIBUTION			
SOIL			
Dry sludge application rate on agricultural soil	0	[kg.ha-1.yr-1]	S
Dry sludge application rate on grassland	0	[kg.ha-1.yr-1]	S
SUBSTANCE			
SUBSTANCE IDENTIFICATION			
General name	Benzoghiperylene		S
Description			D
CAS-No	191-24-2		S
EC-notification no.			D
EINECS no.	205-883-8		S
PHYSICO-CHEMICAL PROPERTIES			
Molecular weight	278.35	[g.mol-1]	S
Melting point	277	[oC]	S
Boiling point	545	[oC]	S
Vapour pressure at test temperature	1.40E-08	[Pa]	S
Temperature at which vapour pressure was measured	25	[oC]	D
Vapour pressure at 25 [oC]	1.40E-08	[Pa]	O
Octanol-water partition coefficient	6.22	[log10]	S
Water solubility at test temperature	0.14	[ug.l-1]	S
Temperature at which solubility was measured	25	[oC]	D
Water solubility at 25 [oC]	0.14	[ug.l-1]	O

PARTITION COEFFICIENTS AND BIOCONCENTRATION FACTORS			
SOLIDS-WATER			
Chemical class for Koc-QSAR	Predominantly hydrophobics		S
Organic carbon-water partition coefficient	1.02E+06	[l.kg-1]	S
AIR-WATER			
Henry's law constant at test temparature	0.027	[Pa.m3.mol-1]	S
Temperature at which Henry's law constant was measured	20	[oC]	S
BIOCONCENTRATION FACTORS			
PREDATOR EXPOSURE			
Bioconcentration factor for earthworms	2.00E+04	[l.kgwwt-1]	S
HUMAN AND PREDATOR EXPOSURE			
Bioconcentration factor for fish	2.83E+04	[l.kgwwt-1]	S
Biomagnification factor in fish	1	[-]	S
Biomagnification factor in predator	1	[-]	S
DEGRADATION AND TRANSFORMATION RATES			
CHARACTARIZATION			
Characterization of biodegradability	Not biodegradable		S
WATER/SEDIMENT			
WATER			
Rate constant for biodegradation in surface water	1.44E-05	[d-1] (12[oC])	S
SEDIMENT			
Total rate constant for degradation in bulk sediment	9.63E-07	[d-1] (12[oC])	S
AIR			
Specific degradation rate constant with OH-radicals	8.69E-11	[cm3.molec-1.s-1]	S
SOIL			
Rate constant for biodegradation in bulk soil	1.44E-06	[d-1] (12[oC])	S
RELEASE ESTIMATION			
CHARACTERIZATION AND TONNAGE			
High Production Volume Chemical	Yes		S
Production volume of chemical in EU	[redacted]	[tonnes.yr-1]	S
USE PATTERNS			
PRODUCTION STEPS			
EMISSION INPUT DATA			

Usage/production title	Formulation of CTPht/AO		S
Emission scenario	no special scenario selected/available		S
INTERMEDIATE RESULTS			
INTERMEDIATE			
RELEASE FRACTIONS AND EMISSION DAYS			
PRODUCTION			
Emission tables	A1.1 (general table), B1.4 (specific uses)		S
RELEASE FRACTIONS			
Fraction of tonnage released to air	[redacted]	[-]	S
Fraction of tonnage released to wastewater	[redacted]	[-]	S
Fraction of tonnage released to industrial soil	0	[-]	S
EMISSION DAYS			
Fraction of the main local source	1	[-]	S
Number of emission days per year	365	[-]	S
REGIONAL AND CONTINENTAL TOTAL EMISSIONS			
Total regional emission to wastewater	0	[kg.d-1]	S
Total regional emission to surface water	5.78E-06	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Bypass STP		S
Use or bypass STP (local marine assessment)	Bypass STP		S
CONFIGURATION			
Effluent discharge rate of this STP	302.57	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	1.12E+06	[m3.d-1]	S
Dilution factor (rivers)	1000	[-]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	2.16E-05	[ug.m-3]	O
Regional PEC in seawater (total)	2.03E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	8.46E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O

Regional PEC in seawater (dissolved)	1.32E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.11E-14	[mg.m-3]	O
Regional PEC in agricultural soil (total)	7.34E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	4.08E-13	[mg.l-1]	O
Regional PEC in natural soil (total)	1.52E-08	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	1.52E-08	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	3.75E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	5.83E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	7.12E-16	[mg.l-1]	O
Continental PEC in seawater (total)	2.90E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	2.78E-16	[mg.l-1]	O
Continental PEC in seawater (dissolved)	1.89E-15	[mg.l-1]	O
Continental PEC in air (total)	2.20E-17	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.45E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	8.05E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	3.00E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.00E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.23E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	8.34E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	2.00E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.30E-15	[mg.l-1]	O
Moderate PEC in air (total)	3.22E-19	[mg.m-3]	O
Moderate PEC in soil (total)	4.39E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	5.76E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.99E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.30E-15	[mg.l-1]	O
Arctic PEC in air (total)	9.25E-20	[mg.m-3]	O
Arctic PEC in soil (total)	1.13E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	5.73E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.83E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.19E-15	[mg.l-1]	O
Tropic PEC in air (total)	6.34E-19	[mg.m-3]	O
Tropic PEC in soil (total)	7.74E-13	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	5.24E-11	[mg.kgwwt-1]	O

STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.011	[%]	O
Steady-state mass fraction in regional seawater	1.15E-03	[%]	O
Steady-state mass fraction in regional air	6.36E-05	[%]	O
Steady-state mass fraction in regional agricultural soil	8.48	[%]	O
Steady-state mass fraction in regional natural soil	1.97	[%]	O
Steady-state mass fraction in regional industrial soil	0.731	[%]	O
Steady-state mass fraction in regional freshwater sediment	2.2	[%]	O
Steady-state mass fraction in regional seawater sediment	0.114	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	3.17E-05	[%]	O
Steady-state mass fraction in continental seawater	0.288	[%]	O
Steady-state mass fraction in continental air	2.18E-05	[%]	O
Steady-state mass fraction in continental agricultural soil	1.46	[%]	O
Steady-state mass fraction in continental natural soil	0.341	[%]	O
Steady-state mass fraction in continental industrial soil	0.126	[%]	O
Steady-state mass fraction in continental freshwater sediment	6.32E-03	[%]	O
Steady-state mass fraction in continental seawater sediment	1.43	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	11	[%]	O
Steady-state mass fraction in moderate air	3.55E-06	[%]	O
Steady-state mass fraction in moderate soil	0.206	[%]	O
Steady-state mass fraction in moderate sediment	11	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	7.19	[%]	O
Steady-state mass fraction in arctic air	5.57E-07	[%]	O
Steady-state mass fraction in arctic soil	0.0231	[%]	O
Steady-state mass fraction in arctic sediment	7.14	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	23.1	[%]	O
Steady-state mass fraction in tropic air	1.14E-05	[%]	O
Steady-state mass fraction in tropic soil	0.356	[%]	O
Steady-state mass fraction in tropic sediment	22.8	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	7.79E-05	[kg]	O
Steady-state mass in regional seawater	8.11E-06	[kg]	O

Steady-state mass in regional air	4.50E-07	[kg]	O
Steady-state mass in regional agricultural soil	0.0599	[kg]	O
Steady-state mass in regional natural soil	0.0139	[kg]	O
Steady-state mass in regional industrial soil	5.17E-03	[kg]	O
Steady-state mass in regional freshwater sediment	0.0155	[kg]	O
Steady-state mass in regional seawater sediment	8.04E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	2.24E-07	[kg]	O
Steady-state mass in continental seawater	2.03E-03	[kg]	O
Steady-state mass in continental air	1.54E-07	[kg]	O
Steady-state mass in continental agricultural soil	0.0103	[kg]	O
Steady-state mass in continental natural soil	2.41E-03	[kg]	O
Steady-state mass in continental industrial soil	8.92E-04	[kg]	O
Steady-state mass in continental freshwater sediment	4.46E-05	[kg]	O
Steady-state mass in continental seawater sediment	0.0101	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0781	[kg]	O
Steady-state mass in moderate air	2.51E-08	[kg]	O
Steady-state mass in moderate soil	1.46E-03	[kg]	O
Steady-state mass in moderate sediment	0.0774	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0508	[kg]	O
Steady-state mass in arctic air	3.93E-09	[kg]	O
Steady-state mass in arctic soil	1.63E-04	[kg]	O
Steady-state mass in arctic sediment	0.0504	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.163	[kg]	O
Steady-state mass in tropic air	8.09E-08	[kg]	O
Steady-state mass in tropic soil	2.52E-03	[kg]	O
Steady-state mass in tropic sediment	0.161	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	7.01E-10	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	7.57E-09	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in surface water (dissolved)	7.57E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	7.72E-04	[mg.kgdwt-1]	O

Local PEC in seawater during emission episode (dissolved)	7.56E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	7.56E-08	[mg.l-1]	O
Local PEC in marine sediment during emission episode	7.71E-03	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	3.16E-07	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	3.22E-07	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	6.26E-07	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.58E-11	[mg.l-1]	O
Local PEC in pore water of grassland	3.07E-11	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.58E-11	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V C.11, OECD 209		S
EC50 for micro-organisms in a STP	??	[mg.l-1]	D
EC10 for micro-organisms in a STP	??	[mg.l-1]	D
NOEC for micro-organisms in a STP	??	[mg.l-1]	D
AQUATIC ORGANISMS			
FRESH WATER			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish	??	[mg.l-1]	D
L(E)C50 for Daphnia	??	[mg.l-1]	D
EC50 for algae	??	[mg.l-1]	D
LC50 for additional taxonomic group	??	[mg.l-1]	D
Aquatic species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish	??	[mg.l-1]	D
NOEC for Daphnia	??	[mg.l-1]	D
NOEC for algae	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
NOEC for additional taxonomic group	??	[mg.l-1]	D
MARINE			
L(E)C50 SHORT-TERM TESTS			
LC50 for fish (marine)	??	[mg.l-1]	D
L(E)C50 for crustaceans (marine)	??	[mg.l-1]	D
EC50 for algae (marine)	??	[mg.l-1]	D

LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
LC50 for additional taxonomic group (marine)	??	[mg.l-1]	D
Marine species	other		D
NOEC LONG-TERM TESTS			
NOEC for fish (marine)	??	[mg.l-1]	D
NOEC for crustaceans (marine)	??	[mg.l-1]	D
NOEC for algae (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
NOEC for additional taxonomic group (marine)	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for fresh-water sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
MARINE SEDIMENT			
L(E)C50 SHORT-TERM TESTS			
LC50 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10/NOEC LONG-TERM TESTS			
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
EC10 for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D

Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
NOEC for marine sediment organism	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested sediment	0.05	[kg.kg-1]	D
TERRESTRIAL ORGANISMS			
L(E)C50 SHORT-TERM TESTS			
LC50 for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
EC50 for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
LC50 for other terrestrial species	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC LONG-TERM TESTS			
NOEC for plants	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for earthworms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for microorganisms	??	[mg.kgwwt-1]	D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
NOEC for additional taxonomic group	??	[mg.kgwwt-1]	D
Terrestrial species	other		D
Weight fraction of organic carbon in tested soil	0.02	[kg.kg-1]	D
BIRDS			
LC50 in avian dietary study (5 days)	??	[mg.kg-1]	D
NOEC via food (birds)	??	[mg.kg-1]	D
NOAEL (birds)	??	[mg.kg-1.d-1]	D
Conversion factor NOAEL to NOEC (birds)	8	[kg.d.kg-1]	D
MAMMALS			
REPEATED DOSE			
ORAL			
Oral NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Oral CED (repdose)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (repdose)	??	[mg.kg-1]	D
LOEC via food (repdose)	??	[mg.kg-1]	D
CED via food (repdose)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (repdose)	??	[mg.m-3]	D
Inhalatory LOAEL (repdose)	??	[mg.m-3]	D
Inhalatory CED (repdose)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (repdose)	??	[mg.kg-1.d-1]	D
Dermal CED (repdose)	??	[mg.kg-1.d-1]	D
FERTILITY			
ORAL			
Oral NOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral LOAEL (fert)	??	[mg.kg-1.d-1]	D
Oral CED (fert)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (fert)	??	[mg.kg-1]	D
LOEC via food (fert)	??	[mg.kg-1]	D
CED via food (fert)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (fert)	??	[mg.m-3]	D
Inhalatory LOAEL (fert)	??	[mg.m-3]	D
Inhalatory CED (fert)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (fert)	??	[mg.kg-1.d-1]	D
Dermal CED (fert)	??	[mg.kg-1.d-1]	D
MATERNAL-TOX			
ORAL			
Oral NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Oral CED (mattox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (mattox)	??	[mg.kg-1]	D
LOEC via food (mattox)	??	[mg.kg-1]	D
CED via food (mattox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (mattox)	??	[mg.m-3]	D
Inhalatory LOAEL (mattox)	??	[mg.m-3]	D
Inhalatory CED (mattox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (mattox)	??	[mg.kg-1.d-1]	D
Dermal CED (mattox)	??	[mg.kg-1.d-1]	D
DEVELOPMENT-TOX			
ORAL			
Oral NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Oral CED (devtox)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (devtox)	??	[mg.kg-1]	D
LOEC via food (devtox)	??	[mg.kg-1]	D
CED via food (devtox)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (devtox)	??	[mg.m-3]	D
Inhalatory LOAEL (devtox)	??	[mg.m-3]	D
Inhalatory CED (devtox)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (devtox)	??	[mg.kg-1.d-1]	D
Dermal CED (devtox)	??	[mg.kg-1.d-1]	D
CARC (THRESHOLD)			
ORAL			
Oral NOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral LOAEL (carc)	??	[mg.kg-1.d-1]	D
Oral CED (carc)	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D

Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
NOEC via food (carc)	??	[mg.kg-1]	D
LOEC via food (carc)	??	[mg.kg-1]	D
CED via food (carc)	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory NOAEL (carc)	??	[mg.m-3]	D
Inhalatory LOAEL (carc)	??	[mg.m-3]	D
Inhalatory CED (carc)	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal NOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal LOAEL (carc)	??	[mg.kg-1.d-1]	D
Dermal CED (carc)	??	[mg.kg-1.d-1]	D
CARC (NON-THRESHOLD)			
ORAL			
Oral T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Oral CED for non-threshold effects	??	[mg.kg-1.d-1]	D
Species for conversion of NOAEL to NOEC	Rattus norvegicus (<=6 weeks)		D
Conversion factor NOAEL to NOEC	10	[kg.d.kg-1]	O
T25 via food for non-threshold effects	??	[mg.kgfood-1]	D
CED via food for non-threshold effects	??	[mg.kgfood-1]	D
INHALATORY			
Inhalatory T25 for non-threshold effects	??	[mg.m-3]	D
Inhalatory CED for non-threshold effects	??	[mg.m-3]	D
Correction factor for allometric scaling	1	[-]	D
DERMAL			
Dermal T25 for non-threshold effects	??	[mg.kg-1.d-1]	D
Dermal CED for non-threshold effects	??	[mg.kg-1.d-1]	D
ACUTE			
Oral LD50	??	[mg.kg-1]	D
Oral Discriminatory Dose	??	[mg.kg-1]	D
Inhalatory LC50	??	[mg.m-3]	D
Dermal LD50	??	[mg.kg-1]	D
PREDATOR			
Duration of (sub-)chronic oral test	28 days		D
NOEC via food for secondary poisoning	??	[mg.kg-1]	O
Source for NOEC-via-food data	No data available, enter manually		S

BIO-AVAILIBILITY			
Bioavailability for oral uptake (oral to inhalation)	0.5	[-]	D
Bioavailability for oral uptake (oral to dermal)	1	[-]	D
Bioavailability for oral uptake (route to oral)	1	[-]	D
Bioavailability for inhalation (route from inhalation)	1	[-]	D
Bioavailability for inhalation (route to inhalation)	1	[-]	D
Bioavailability for dermal uptake (route from dermal)	0.1	[-]	O
Bioavailability for dermal uptake (route to dermal)	0.1	[-]	O
ENVIRONMENTAL EFFECTS ASSESSMENT			
ENVIRONMENTAL PNECS			
FRESH WATER			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Aqua	0.082	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Aqua	10	[-]	S
PNEC for aquatic organisms	8.20E-03	[ug.l-1]	O
INTERMITTENT RELEASES			
Toxicological data used for extrapolation to PNEC Aqua	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC Aqua	??	[-]	O
PNEC for aquatic organisms, intermittent releases	??	[mg.l-1]	O
STATISTICAL			
PNEC for aquatic organisms with statistical method	??	[mg.l-1]	D
MARINE			
Same taxonomic group for marine LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Marine	0.082	[ug.l-1]	S
Assessment factor applied in extrapolation to PNEC Marine	100	[-]	S
PNEC for marine organisms	8.20E-04	[ug.l-1]	O
STATISTICAL			
PNEC for marine organisms with statistical method	??	[mg.l-1]	D
FRESH WATER SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (fresh)	0.082	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (fresh)	??	[-]	O
PNEC for fresh-water sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for fresh-water sediment organisms (equilibrium partitioning)	0.836	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in fresh-water sediment?	Yes		S
PNEC for fresh-water sediment, normalised to 10% o.c. (local)	0.836	[mg.kgdwt-1]	O

PNEC for fresh-water sediment, normalised to 5% o.c. (regional)	0.836	[mg.kgdwt-1]	O
MARINE SEDIMENT			
Toxicological data used for extrapolation to PNEC sediment (marine)	0.082	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC sediment (marine)	??	[-]	O
PNEC for marine sediment organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for marine sediment organisms (equilibrium partitioning)	0.0836	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in marine sediment?	Yes		S
PNEC for marine sediment, normalised to 10% o.c. (local)	0.0836	[mg.kgdwt-1]	O
PNEC for marine sediment, normalised to 5% o.c. (regional)	0.0836	[mg.kgdwt-1]	O
TERRESTRIAL			
Same taxonomic group for LC50 and NOEC	No		O
Toxicological data used for extrapolation to PNEC Terr	0.082	[mg.kgdwt-1]	S
Assessment factor applied in extrapolation to PNEC Terr	??	[-]	O
PNEC for terrestrial organisms (from toxicological data)	??	[mg.kgdwt-1]	O
PNEC for terrestrial organisms (equilibrium partitioning)	0.167	[mg.kgdwt-1]	O
Equilibrium partitioning used for PNEC in soil?	Yes		S
PNEC for terrestrial organisms	0.167	[mg.kgdwt-1]	O
STATISTICAL			
PNEC for terrestrial organisms with statistical method	??	[mg.kgdwt-1]	D
SECONDARY POISONING			
Toxicological data used for extrapolation to PNEC oral	??	[mg.kg-1]	O
Assessment factor applied in extrapolation to PNEC oral	??	[-]	O
PNEC for secondary poisoning of birds and mammals	??	[mg.kg-1]	O
STP			
Toxicological data used for extrapolation to PNEC micro	??	[mg.l-1]	O
Assessment factor applied in extrapolation to PNEC micro	??	[-]	O
PNEC for micro-organisms in a STP	??	[mg.l-1]	O
RISK CHARACTERIZATION			
ENVIRONMENTAL EXPOSURE			
LOCAL			
RISK CHARACTERIZATION OF [PRODUCTION]			
WATER			
RCR for the local fresh-water compartment	9.23E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	0.0922	[-]	O
RCR for the local fresh-water compartment, statistical method	??	[-]	O

RCR for the local marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the local fresh-water sediment compartment	9.23E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	0.922	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.89E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
PREDATORS			
RCR for fish-eating birds and mammals (fresh-water)	??	[-]	O
RCR for fish-eating birds and mammals (marine)	??	[-]	O
RCR for top predators (marine)	??	[-]	O
RCR for worm-eating birds and mammals	??	[-]	O
REGIONAL			
WATER			
RCR for the regional fresh-water compartment	1.03E-06	[-]	O
RCR for the regional marine compartment	1.61E-06	[-]	O
RCR for the regional fresh-water compartment, statistical method	??	[-]	O
RCR for the regional marine compartment, statistical method	??	[-]	O
SEDIMENT			
RCR for the regional fresh-water sediment compartment	2.06E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	3.20E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	4.97E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional soil compartment, statistical method	??	[-]	O

21 ANNEX X – PHOTOS

21.1 Sampling system for pitch mixtures

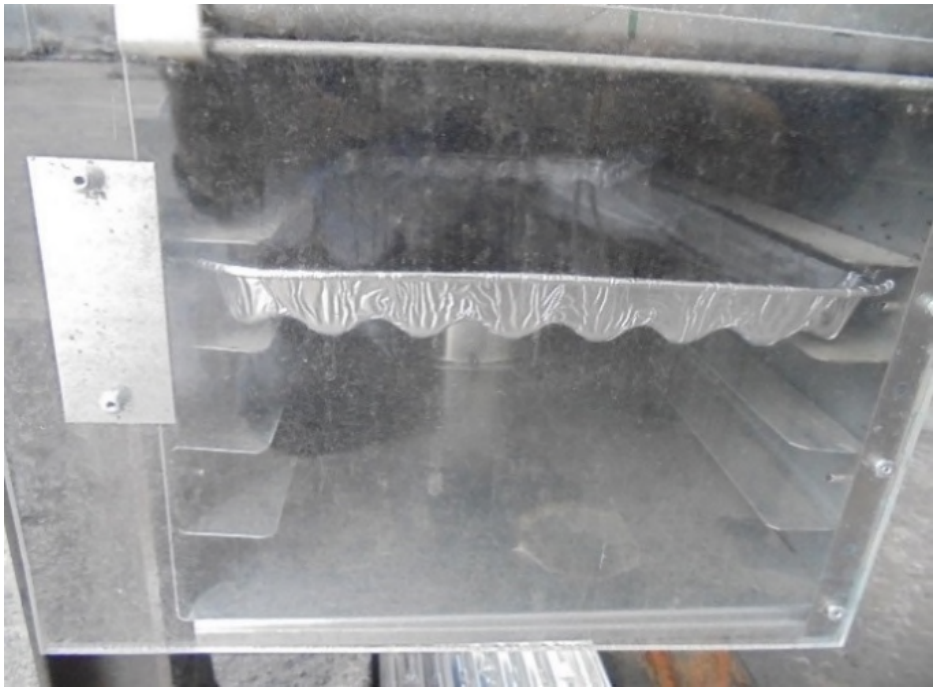


Figure: **Fully closed pitch sampling box with filled sampling container (closed)**

Figure: **Fully closed pitch sampling box with sampling container (closed) with a sign indicating that a respiration mask needs to be worn when opening the sampling box**

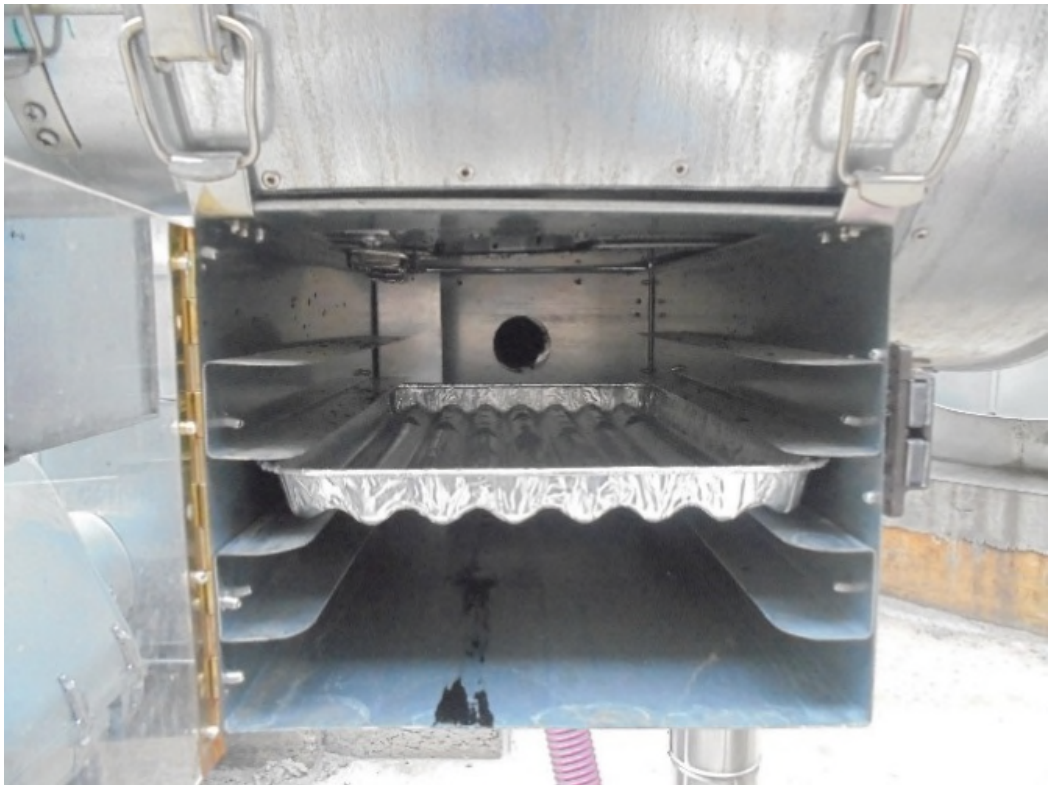


Figure: **Fully closed pitch sampling box with sampling container (open)**

Figure: **Pitch sampling container**

Figure: **Fully closed pitch sampling box equipped with local ventilation and cleaning of the extracted air on an active carbon adsorbent**

Figure: **New pitch sampling container, closed, with pictograms**

21.2 Sample reception box in the laboratory

Figure: Sample reception box in laboratory

22 ANNEX XI – BIOMONITORING DATA

22.1 Methods

Biomonitoring – method of analysis

The aim of the biomonitoring campaign is to detect the exposure of workers to polycyclic aromatic hydrocarbons (PAH) in the factory. Therefore the amount of 1-hydroxypyrene in urine is determined. 1-hydroxypyrene is a metabolite of pyrene, a component of PAH mixtures. The half-life of 1-hydroxypyrene in urine is 18-20 h on average, which means that 90% of the amount of hydroxypyrene present in urine originates from an exposure of the last two (working) days.

For the biological monitoring a sample of the urine is collected at specific moments: every time at the start and the end of a shift, both at the beginning and the end of a work week:

- Day 1, start of the work week, before the start of the shift
- Day 1 after the end of the shift
- Day 5, end of the work week, before the start of the shift
- Day 5, after the end of the shift

At each of these moments a urine sample was requested from the people in civil clothes to avoid contamination by the working clothes. On the days of sampling every employee is asked to fill in a questionnaire to gather information regarding the tasks the person has performed during the monitoring, the PPE's that were used, smoking habits, personal hygiene and the use of PAH-containing products at home.

Samples are analysed by AML, a toxicological lab in Antwerp, Belgium. As a reference substance, 1-hydroxyperene is measured. The concentration of 1-hydroxyperene is expressed as µg/g creatinine to account for dilution of the urine sample. The concentration of 1-hydroxypyrene in urine is different in people that are professionally exposed to PAH, and is different in smokers versus non-smokers.

Of a sample of 10 mL of urine that is collected, 50 µL is prepared and loaded for analysis in a HPLC-tandem mass spectrometry after enzymatic hydrolysis and removal of the precipitation after centrifugation.

ANALYSE: **1-Hydroxypyreen (U)**

(*) Extra info voor u/uw profiel

Analyse nummer (*)	57900
Opvraag nummer (*)	57902

Details (3)

Labo	Analyse	AL	Rap	Omschrijving Analyse	Staaltype	Eenheid BE	Eenheid NL	LOINC NL	I/O	Srt	Len	DecBE	DecNL
2	26801	N	Y	Creatinine		mg/dl	µmol/L	14683-7	B,O	3	5	0	0
2	57901	N	Y	1-Hydroxypyreen	UH	µg/l	µmol/L			3	6	2	4
2	57902	N	Y	1-Hydroxypyreen	UH	µg/g creatinine	µmol/mol creat.			3	6	2	2

Uitvoerend labo (*)	A.M.L. Arbeidsgeneeskunde, Toxicologie en Gerechtelijke Analyses (*) Emiel Vloorsstraat 9, 2020-Antwerpen, België 2de verdieping (*)
Labo afdeling (*)	HPLC TEL: HMLT 2835, KB/PATH/MB 2872/2885 Email: KB/PATH/MB info@aml-lab.be
Labo website (*)	www.aml-lab.be
Verstrekker (initialen) (*)	Marc Uytterhoeven (MU - 999023)
Classificatie	Humane analyse
Accreditatie (Belac)	Neen
Ext. Quality Control	Neen
Staaltype 1	Urine (einde laatste werkdag van de week) (U)
Volume/Gewicht (test) (*)	50 µL (het minimum volume/gewicht vereist om de analyse welgeteld één maal uit te voeren)
Volume/Gewicht (dood) (*)	50 µL (het minimum volume/gewicht dat een toestel extra vraagt om de analyse zeker te kunnen uitvoeren, zonder rekening te houden met het eigenlijke test volume)
Volume/Gewicht labo (*)	100 µL (de som van volume/gewicht test + volume/gewicht dood)
Volume/Gewicht	10 mL (het volume/gewicht dat het laboratorium vraagt aan de klant waarbij rekening wordt gehouden met eventuele controle en/of titratie)
Toestel (*)	AB Sciex Triple Quad 5500
Methode	Tandem massa spectrometrie
Frequentie	1x per week (aantal keren dat een analyse wordt ingezet in een bepaalde periode)

22.2 Results

For details see separate file „Confidential information 20190207 report on biomonitoring results.pdf” attached to IUCLID section 13.

23 ANNEX XII – PAH EMISSIONS FROM THE FOUR RELEVANT SCRUBBERS – EMISSIONS FROM 2018 AND APPLIED REDUCTION FACTORS FOR THE 4 EFSA PAHS

Table: PAH emissions from the four relevant scrubbers – emissions from 2018 and applied reduction factors [kg/y] for the 4 EFSA PAHs

	K101				K102				K100A				31B101				Sum of 4 scrubbers	Sum of 4 scrubbers incl. reduction
		Measured	Value used	Emission reduced by 80%		Measured	Value used	Emission reduced by 80%		Measured	Value used	Emission reduced by 99%		Measured	Value used	Emission reduced by 80%	Emission	Reduced emission
Benzo[a]anthracene	<	0.0001	0.0001	0.0000		0.0029	0.0029	0.0006		0.0014	0.0014	0.0000		0.0000	0.0000	0.0000	0.0044	0.0006
Chrysene	<	0.0001	0.0001	0.0000		0.0021	0.0021	0.0004		0.0007	0.0007	0.0000		0.0000	0.0000	0.0000	0.0029	0.0004
Benzo[a]pyrene	<	0.0001	0.0001	0.0000		0.0002	0.0002	0.0000		0.0005	0.0005	0.0000	<	0.0000	0.0000	0.0000	0.0007	0.0001
Benzo[b]fluoranthene	<	0.0001	0.0001	0.0000		0.0005	0.0005	0.0001		0.0010	0.0010	0.0000	<	0.0000	0.0000	0.0000	0.0016	0.0001
4 EFSA PAHs (sum of 4)																	0.0095	0.0012
Flow * (Nm^3/h)				20 [1]				20 [1]				14 [2]				25		
Possible scaling factors	51% of the time fully open, 23% of the time fully closed				2% of the time fully open, 73% of the time fully closed				67% of the tank farm volume contains AFA formulations with AO.									
PAH reduction program planned	2019: post-treatment on activated carbon (>80% yield)				2019: post-treatment on activated carbon (>80% yield)				2019: connection to thermal incinerator of the tar refinery (99-				2019: post-treatment on activated carbon (>80% yield)					

actions			100% yield)			
In case that emission data was provided with "<", the given value was divided by 2 (considering LOD/2 for the measured concentration). [1] Flowrates below the measuring range of the equipment have been determined using process data. [2] Average 2018 flowrate.						

24 ANNEX XIII – PEC_{ORAL}, PEC_{AIR} AND ELCR VALUES FOR THE LOCAL AND REGIONAL ASSESSMENT OF HVE WITH AIR EMISSION DATA FROM 2018

Table: Local PEC_{oral} and PEC_{air} (obtained from EUSES modelling with air emission data from 2018), used for calculation of excess life cancer risks (ELCRs)

Exposure route	Explanation	Benzo[a]-pyrene	Chrysene	Benzo[b]-fluoranthene	Benz[a]-anthracene	Sum PAH4 EFSA	Risk estimate for cancer per ng PAH4/kg bw/day	Risk estimate for cancer per 1 ng BaP/m³ (excess lifetime cancer risk)		ELCR
Oral general population	Total daily intake oral (PEC_{oral}) for individual PAHs [ng/kg/d]	3.37E-03	6.17E-02	2.86E-01	2.03E-02					
	Total daily intake oral (PEC_{oral}) for sum PAH4 EFSA [ng/kg/d]					3.71E-01	2.06E-06			**7.65E-07**
Inhalation general population	Annual average local PEC in air (total) [ng/m³]	4.03E-05						lung	3.00E-05	**1.21E-09**
								bladder	2.10E-05	**8.46E-10**
								total (lung & bladder)		**2.06E-09**
Workers onsite (not involved in formulation activities)	Annual average local PEC in air (total) [ng/m³]	4.03E-05						lung	5.60E-06	**2.26E-10**
								bladder	4.00E-06	**1.61E-10**
								total (lung & bladder)		**3.87E-10**

Table: **Regional PEC_{oral} and PEC_{air} (obtained from EUSES modelling with air emission data from 2018), used for calculation of excess life cancer risks (ELCRs)**

Exposure route	Explanation	Benzo[a]-pyrene	Chrysene	Benzo[b]-fluoranthene	Benz[a]-anthracene	Sum PAH4 EFSA	Risk estimate for cancer per ng PAH4/kg bw/day	Risk estimate for cancer per 1 ng BaP/m^3 (excess lifetime cancer risk)		ELCR
Oral general population	Total daily intake oral (PEC_{oral}) for individual PAHs [ng/kg/d]	3.84E-06	7.48E-05	3.11E-04	3.79E-06					
	Total daily intake oral (PEC_{oral}) for sum PAH4 EFSA [ng/kg/d]					3.93E-04	2.06E-06			**8.10E-10**
Inhalation general population	Regional PEC in air (total) [ng/m^3]	1.79E-09						lung	3.00E-05	**5.37E-14**
								bladder	2.10E-05	**3.76E-14**
								total (lung & bladder)		**9.13E-14**