CHEMICAL SAFETY REPORT

Legal name of applicant(s):	RÜTGERS Germany GmbH
Submitted by:	RÜTGERS Germany GmbH
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 section 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, 2009a), 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, 2009b; c).

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, 2009b; c).

The nine PAHs considered as PBT and/or vPvB substances in the SVHC Support Document for CTPht (ECHA, 2009a) 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, 2009a)

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, 2009a).

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, 2009a; 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]	1.7×10^{-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 Kow were preferably based on slow-stirring/generator column (c) or slow-stirring methods (d) using average values. If absent the log Kow 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, 2017) 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 1 ng BaP/m^3 (40 years of occupational exposure) Bladder tumours: 4×10^{-6} per 1 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 follows the equation as given by RAC (ECHA, 2018). It 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 some exposed worker groups, for which no biomonitoring data were available.

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 well above 120 °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

The main activity of RÜTGERS Germany GmbH at its production site Kekuléstr. 30, Castrop-Rauxel, North Rhine-Westphalia, Germany, is the distillation 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).

Currently, the larger part of the production volume of CTPht at the site (<[redacted] (50 000-500 000) t per year) is sold as neat substance e.g. for production of prebake electrodes for aluminium smelters or production of graphite electrodes. These uses are exempted from authorisation as intermediate uses and not further considered in this application for authorisation. It is also used as intermediate for production of another substance (which is not subject of authorisation) onsite and thus these amounts are also outside the scope of authorisation. A certain amount is mixed with other streams of the coal tar distillation (so called inline-blending) and put on the market as mixtures. These mixtures are also used in electrode production or as carbon black feedstock. Both uses are considered intermediate uses. The production of these mixtures is subject to this AfA (total volume of CTPht used: [redacted] (1 000-10 000) tonnes per year (PÖ-Mix) for electrode production,[redacted] (5 000-100 000) tonnes CTPht per year (Ölbetrieb) for carbon black feedstock; for details see also Table 9-10).

In the upcoming years there will be more CTPht formulations (i.e.so called [redacted], see also Table 9-10) produced at RÜTGERS Germany. To consider this circumstance the larger part of the production volume is considered relevant for this AfA (total of up to [redacted] (25 000-400 000) t per year).

The production volume of AO is around [redacted](10 000-100 000) t per year. The largest part of AO is formulated and then sold as carbon black feedstock (CBO[redacted]). Use of AO in carbon black feedstock is considered an intermediate use and therefore outside of the scope of authorisation. A minor quantity of AO produced (approx. [redacted] (100-5 000) t AO per year; [redacted] (100-2 500) t in PÖ-Mix, [redacted] (100-2 500) t in Ölbetrieb) is used for mixing with other production streams and will be used for products used as intermediates. The production of these mixtures is also subject to this AfA (for details see

Table 9–11). The remaining quantity of AO is used for producing EU creosote (CAS 8001-58-9). Upstream formulation and use of EU creosote is exempted from authorisation (see also ECHA Q&A 1027).

The formulation activities involving CTPht and AO which are subject of this AfA take place in Castrop-Rauxel in dedicated facilities called

- PÖ-Mix (formulation of CTPht with either AO or other production streams, approx. [redacted](100-10 00) t CTPht per year, and approx. [redacted] (100-2 500) t AO per year) and
- Ölbetrieb (formulation of AO with other production streams, up to [redacted] (10 000-100 000) t AO per year; formulation CTPht potentially up to approx. [redacted] (5 000-100 000)t CTPht per year)

For this assessment maximum potential tonnages of AO and CTPht for CBO production in Ölbetrieb are used. In reality, if high amounts of AO are used then the required CTPht amount will be lower and vice versa.

A subsequent product of CTPht is CTPht heat treated ([redacted]), which is kept in another dedicated facility, i.e. [redacted] unit (which is part of EPT), in which also formulation processes with AO occur.

- [redacted] unit (formulation of [redacted] with either AO or other production streams[redacted] (1-1 000) t AO per year).

Table 9-10 and Table 9–11 provide an overview on the types of formulations. All mixtures containing CTPht are today marketed in the EEA and are destined for use in the carbon/graphite industry and potentially in carbon black feedstock production (CBO, “carbon black oil”). AO is mainly used for producing carbon black feedstock, which is used inside the EEA.

Table 9-10: Tonnages and use area for mixtures containing CTPht

Mixture type	Tonnage CTPht (t/y)	Export out of EEA (t/y)	Used in EEA (intermediate uses) (t/y)
CTPht + AO and/or other oil streams (PÖ-Mix)	[redacted] (25 000-400 000) Other products: [redacted] (100-10 000)	none none	all all
CTPht + other oil streams (Ölbetrieb)	CBO: [redacted] (5 000-100 000)	CBO: none	CBO: all

Table 9-11: Tonnages and use area for mixtures containing AO

Mixture type	Tonnage AO (t/y)	Export out of EEA (t/y)	Used in EEA (intermediate uses) (t/y)
AO with CTPht (PÖ-Mix)	Other products: [redacted] (100-2 500)	none	all
AO mixtures (Ölbetrieb)	CBO: [redacted] (10 000-100 000) Other products: [redacted] (100-2 500) EU Creosote (exempted): [redacted] (10 000-100 000)	CBO: none Other products: none EU Creosote (exempted): [redacted] (1-50)% of product	CBO: all Other products: all EU Creosote (exempted): [redacted] (50-100)% of product
[redacted] mixtures with AO ([redacted] unit)	[redacted] (1-1 000)	all	none

CBO = carbon black oil

The dedicated facilities in which all formulation processes occur, PÖ-Mix, Ölbetrieb and the [redacted] unit, are all located in the northern part of the site (see Annex I – Site plan). PÖ-Mix and [redacted] unit are in close proximity and are combined in the so called [redacted])). [redacted] consists of a facility with [redacted] (1-20) tanks and the [redacted] unit consist of [redacted] (1-30) tanks. The units of [redacted] relevant for AO/oil mixtures consists of the tank farms called [redacted] with a total of approx [redacted] (5-60) tanks. The quantity of CTPht mixtures coming from [redacted] is handled in [redacted] with a total of [redacted] (5-30) tanks. All of the tanks are located in concrete tank pits (secondary containment).

The dedicated filling stations for tank trucks for the formulations of PÖ-Mix are also located in the northern part of the site [redacted]

Mixtures from Ölbetrieb are loaded via the central oil loading facility, which is located nearby ([redacted]). This central oil loading facility is a roofed outdoor plant and consists of [redacted] (3-15) truck loading / container loading / extraction points and a rail tank car loading / extraction point.

Mixtures containing CTPht coming from Ölbetrieb (i.e. carbon black feedstock) are also transported out of the facility via the so called liquid port, which is also situated in the northern part of the site ([redacted]).

Relevant [redacted] formulations are conducted to a dedicated drum filling station, which is located in the southeast of the site ([redacted]). Specific products containing AO from the [redacted] unit are transported there in rail tank cars. A new IBC filling station will be opened in the northern area ([redacted]) soon.

9.1.1.2 Process description

CTPht and AO obtained from distillation of coal tar are stored in tanks of the EPT (combines PÖ-Mix and [redacted] unit) or Ölbetrieb units. Through dedicated closed lines other materials are added batch-wise or by inline-blending to obtain the desired composition of the mixture. Process temperatures are up [redacted] without CTPht. For [redacted] mixed [redacted] with AO process temperatures are around [redacted]. The distillation of coal tar (production called continuous tar distillation, KTD) runs 24 hours, 7 days per week (apart from a general shut-down [redacted] per year for maintenance). The KTD shut-down has no significance for the formulation activities as storage tanks are filled before the shut-down of the production facility and thus formulation activities continue throughout the maintenance of the production facility.

The whole formulation process is highly automated and run by operators in the control room without presence of operators close to the tanks ("Prozessleitsytsem", PLS; automated mixing, manual mixing not foreseen). There are various technical implementations, which guarantee mixing processes without emissions. There are common technicalities to all facilities and specificities for certain groups of the tank farms from Ölbetrieb and the EPT (see 9.1.1.4 and 9.1.1.5 for detail).

In general

- All tanks are equipped with exhaust pipes on the top, which constantly suck out the exhaust air, which is gathered from all tanks and incinerated on-site (for details see 9.1.1.5).
- The whole process is waterless (for percolating water see 9.1.1.5).

Final products are pumped from the tanks via closed lines to dedicated filling stations for tank trucks (PÖ-Mix and Ölbetrieb (also rail tank cars)), to the liquid port (Ölbetrieb) or are transported by railcar on-site to the drum filling station (relevant products from [redacted] unit).

PÖ-Mix tanks are occasionally emptied [redacted]. The emptying [redacted] can be done in two ways. Either via the suction side of the respective container pump or via a chain slide in the pressure line. Furthermore, the ball valve of the PÖ-Mix must be opened on the slop system itself. Residuals are piped (closed) to other tanks. There is no possibility for exposure.

<u>Handling materials from customer complaints:</u>

Every two or three months one tank truck is returned to the facility. Product returns can occur in case of customer complaints. These trucks (sometimes containing relevant CTPht/AO mixtures) can be drained via the slop system. PÖ-Mix operators are performing these operations. A flexible pipe is connected to the drain port of the tank. Under vacuum the tank can be drained, for this ventilation of the tank truck to be emptied has to be opened. The flexible pipe is removed from the tank truck under vacuum and with an open slide, thus residuals can be removed (no exposure to residuals possible). The slop system [redacted] is discharged to tank group 4. In order for [redacted] to be emptied, the vacuum pump is turned off and the container embroidered. The container can then be disposed of via the sloping line to the [redacted] for quality adjustment. There is no waste.

9.1.1.3 Definition of groups of exposed humans

A) Workers at the PÖ-Mix facility

Operators:

Operators are responsible for performing all tasks in the PÖ-Mix unit: Monitoring of the process and steering activities from the central control room ([redacted], via process control system (PLS)), truck clearance, inspections in the tank area, sampling (only in early and late shift) and analysis at a dedicated lab room adjacent to the control room, documentation.

There is one operator per shift in the PÖ-Mix unit, work is organised

- From Monday to Saturday in 8 h – 3 shifts per day
- On Sunday in 12 h – two shifts per day.

There are 12 workers principally working as PÖ-Mix operators. They are changing shifts with work in another adjacent unit ([redacted] unit) on a weekly basis. All workers are regularly switching between the two units to retain expertise to do both jobs. (Workers in the Ölbetrieb unit are not switching between units).

Operators typically spend up to 3 hours outside (main activities: survey of technical infrastructure, sampling; i.e. activities with potential exposure, but no direct contact to dangerous substances intended) and approx. 5 hours in the central control room (with no direct contact to dangerous substances).

Foremen ("Anlagenvorarbeiter"):

Foremen are working in the same shift system as operators. There are 6 foremen in total (1 per shift) supervising work in all units in the northern part of the production site. They are mainly working inside the central control room with occasional inspections of various places in the northern part of the site.

Their time outdoors close to the PÖ-Mix tank area or the dedicated filling stations is estimated to be around 5% of their shift (i.e. 30 min per shift).

Others:

Other workers (n=4) related to PÖ-Mix unit are supervisors ("Anlagenmeister", n=2), one technician, and one head of operation, all working in the northern part in day shifts (8 h/d, 5 d/w). Mostly their work is inside the control room or relevant other buildings on the facility. Occasionally they perform inspections of the activities performed and technical equipment outside.

Their time outdoors close to the PÖ-Mix tanks area or the dedicated filling stations is estimated to be around 5% of their shift (i.e. 30 min per shift).

B) Workers at the Ölbetrieb facility

Mostly formulations containing AO/and other oils are handled by the operators of Ölbetrieb. Yet they might also handle carbon black feedstock containing CTPht in the future and thus activities leading to human exposure have to be considered as well. Such products containing CTPht are handled in oil storage 6 only.

Operators:

Operators are responsible for performing all tasks in the Ölbetrieb unit: Monitoring of the process and steering activities from the central control room ([redacted], via process control system (PLS), e.g. formulation processes, loading operations at central oil loading or liquid port), truck clearance, inspections in the tank areas, sampling (only in early and late shift) and documentation.

The employee is responsible for the operation of the storage containers and the associated plant components. Sometimes besides steering via the PLS this includes the on-site realization of the product routes for an operational production process. For this purpose, valves (e.g. product flaps, slides, ball valves, etc.) are manipulated and pumping operations performed. He wears the prescribed PPE (see 9.1.1.4, PPE for tasks outside in tank farm).

There is one operator per shift in the Ölbetrieb, work is organised

- From Monday to Saturday in 8 h – 3 shifts per day
- On Sunday in 12 h – two shifts per day.

There are 6 workers principally working as Ölbetrieb operators.

Operators typically spend up to 4 hours outside (main activities: survey of technical infrastructure, sampling (approximately up to 30 minutes), logistics (way to and from the sampling points, way to and from the central laboratory); i.e. activities with potential exposure, but no direct contact to dangerous substances intended) and approx. 4 hours in the central control room (with no direct contact to dangerous substances).

Foremen (“Anlagenvorarbeiter”):

Description of work is already presented above (in section A - Description of groups of exposed workers at the PÖ-Mix facility).

Their time outdoors close to the Ölbetrieb tanks area or the dedicated filling stations is estimated to be around 5% of their shift (i.e. 30 min per shift).

Others:

Other workers (n=4) related to Ölbetrieb are supervisors (“Anlagenmeister”, n=2), one technician, and one head of operation, all working in the northern part in day shifts (8 h/d, 5 d/w). As these are the same personnel as for PÖ-Mix description of their work is already presented above (in section A - Description of groups of exposed workers at the PÖ-Mix facility).

Their time outdoors close to the oil storage tanks area or the dedicated filling stations is estimated to be around 5% of their shift (i.e. 30 min per shift).

C) Loading operators

There are 6 loading operators responsible for loading operations at the PÖ-Mix loading station **and** the central oil loading facility. For loading operations there are two persons involved at each operation:

- Truck driver (no exposure):

The truck driver is in charge of opening the manhole on top of the empty truck. All other tasks are performed by the loading operator. After opening the manhole the truck driver is obliged to retreat to an observation station in about 20 m distance. Truck drivers are dressed according to the transport of dangerous goods regulations (ADR).

- Loading operator:

In each loading operation first, a visual inspection of the condition of the tank car (seals, closures, load capacity, volume, heating, etc.) is performed. The loading operator enters the loading station. The interior of the container is inspected for cleanliness through the opened manhole on top of the road truck (duration approx. 2 min.). The dripping container is removed from the loading arm[1]. Afterwards by hydraulic remote control the loading arm with nozzle is maneuvered onto the manhole. The loading arm is equipped with exhaust ventilation to prevent emissions to air (operation requires approx. 3 min).

Then the operator leaves the loading station. Automatic filling is started from inside the central control room (loading only possible if security chain is activated). Loading of one truck typically requires 1 hour. After the tank is filled, the operator removes the loading arm by remote control out of the manhole. The nozzle is lifted for allowing drops to fall into the tank (200 seconds waiting period required). An emptying of filling line on-site happens automatically on the container [redacted]. The dripping container is positioned and the loading arm is then moved to its resting position (operation requires approx. 5 min). Exhaust ventilation via the [redacted]) is used to extract the exhaust gases of the loading stations and thus prevents emission to air.

During these activities, the staff / truck driver (according to transport of dangerous goods regulations, ADR) will wear basic PPE and in addition, gloves according to the glove plan. After completed loading the RÜTGERS Germany loading operator will wear also a respirator for closing the manhole (full mask) with ABEK filter or respirator with hose.

D) Special activity: barge (ship) loading at the liquid port

This specific activity involves an operator or foreman from Ölbetrieb and, in addition, one worker from the Rütgers fire brigade.

Mixtures from the tank farms are pumped via pipe routes to the liquid port. Essentially, the loading system consists of a loading arm, the product distribution system and all ancillary equipment such as piping, fittings, hydraulic control and condensate water pump. Loading of barges takes generally approx. 4 to 5 hours (approx. 250 to 300 t/h). Depending on water level up to 1000-1200 tonnes are loaded per ship (low water only around 500-600 t). However tasks associated with potential exposure take only a few minutes. In general [redacted], but only a minor fraction of the mixtures thereof contains CTPht.

The member of the RÜTGERS fire brigade provides the loading arm. This is connected by the ship's crew. After connecting the loading arm and before starting the loading process, the ship's crew member must leave the danger area so that a distance of 3 m to the flange connection between the ship and the loading arm is maintained. Under the loading arm, a drip pan is situated under the flange during the entire loading process. This is compulsory for

[1] Full container is closed and transported to waste intermediate storage (AZL) and is subsequently disposed of. There are no cleaning or similar activities.

every ship according to the ADN checklist (ADN = European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways). The drip pan is emptied by the barge's crew in case any residue remains (see below).

The **operator or foreman** from Ölbetrieb is in charge to document the process with signature and to open the slipcase.

The process has suction via the exhaust line (exhaust gas combustion facility, AVS).

Additional safety precautions taken are, e.g. camera surveillance of the process, general surveillance via process control system (PLS), Emergency Stop in central control room, ADN Checklist, and a detailed work instruction ("Betriebsanleitung -Ölverladearm zur Be- und Entladung von Schiffen am Flüssighafen") is provided. Possible equipment leaks due to corrosion / wear / aging are detected during regular plant controls, especially during operation. The trained personnel will immediately report to the shift supervisor and possibly the fire department. All workers wear general PPE (helmet, gloves, safety shoes, work clothes, but no mask).

After loading, the lines are blown with nitrogen to remove residue. If additional residues remain in the pipe, they will be transferred to the drip pan of the barge in the next charging process. Disposal will be performed by barge's crew.

E) Laboratory workers

The central laboratory facility is currently divided in three sections (however there will be restructuring in the near future). In general, workers of all sections are in contact with CTPht/oil and CTP/AO formulations during their work. The sections currently are:

- „A-Seite" (or "laboratory BA"), consists of 5 laboratory workers working on day shift only (8 h/day, 5 days/week)
  - Performing standard analytics (i.e. distillation, grinding, SP (softening point), TI / QI (toluene / quinoline insoluble), Alcan coking value, flash point (closed and open cup), viscosity and filtration rate) according to national or international standards
  - Selected standard analytics is performed on each sample provided from production facility, thus exposure to CTPht/oil and CTP/AO formulations may occur dependent of relative amount of these formulations on the total production volume →i.e. < 5% [redacted]
- „C-Seite", consists of 7 laboratory workers working on night and late shift (8 h/day, 5 days/week)
  - Works performed with relevant formulations are measurements of viscosity
  - Thus 1 laboratory worker per shift will be exposed for 1 hour in case a relevant sample is provided
- 3rd section: 3 additional laboratory workers, on day shift (8 h/day, 5 days/week)
  - Works performed: Determination of BaP by HPLC, determine RFA, wetting and determination of nitrogen content
  - In case relevant sample is analysed – exposure of 1 laboratory worker per shift for 1 hour

Work takes place in fume cupboards. All laboratory workers wear gloves according to the glove plan and required PPE (safety goggles, work clothing). In case of recovery of solid samples a dust mask is worn.

Any waste is disposed in the so-called pitch container, which goes to waste intermediate storage (AZL) and is subsequently disposed of (incineration).

F) Maintenance workers

Maintenance workers are located in the central part of the site, are responsible for maintenance activities at the complete production site and are requested in case of breakdown of pumps etc. in the different units of the RÜTGERS Germany site. Tasks to be performed by the maintenance workers are:

- maintenance on machines and other components
- disassembly and assembly of electrical components
- opening systems
- replacement of apparatus and fittings
- disassembly / assembly of machines
- insulation works
- scaffolding, and
- cleaning.

In total there are 60 maintenance workers at this site. They are divided in supervisor (Meister), foreman or coordinator and workman. In addition workers from external companies (contractors) are required in case specific maintenance work would be required or the workforce has to be increased (e.g. for cleaning operations via vacuum trucks). In general the workers are divided into three groups according to their tasks and skills:

- Contractor coordination within maintenance (FKR)
- Mechanical workshop (MW; machine and pump technology)
- Electro technical workshop (EMR; company electrician, measuring and control technology and communication technology)

RÜTGERS Germany workers of maintenance are organised in two shifts – early and late shift on five days per week. In the early shift there are at least one foreman from each workshop (MW and EMR) and one coordinator for contractors. In the late shift there is at least one coordinator and six workmen.

<u>PÖ-Mix / Ölbetrieb</u>

At the PÖ-Mix / Ölbetrieb facility each day a maintenance job is performed and around 2 to 4 maintenance workers are involved (usually only Monday until Friday, i.e. ~220 days per year). On basis of the very different tasks performed by the maintenance workers estimation of time close to the PÖ-Mix / Ölbetrieb tanks or the dedicated filling stations is difficult. Task durations vary from a few minutes to whole shift length.

G) Description of groups of humans exposed via the environment

Approximately 450 staff members of RÜTGERS Germany are regularly working on the site. On its northeastern and southwestern limits the production site is adjacent to the community of Castrop-Rauxel (approximately 75 000 inhabitants), which is part of the metropolitan region Ruhr (with about 5.1 million inhabitants spread on approximately 4 400 square kilometres, see Figure 9-1 below).

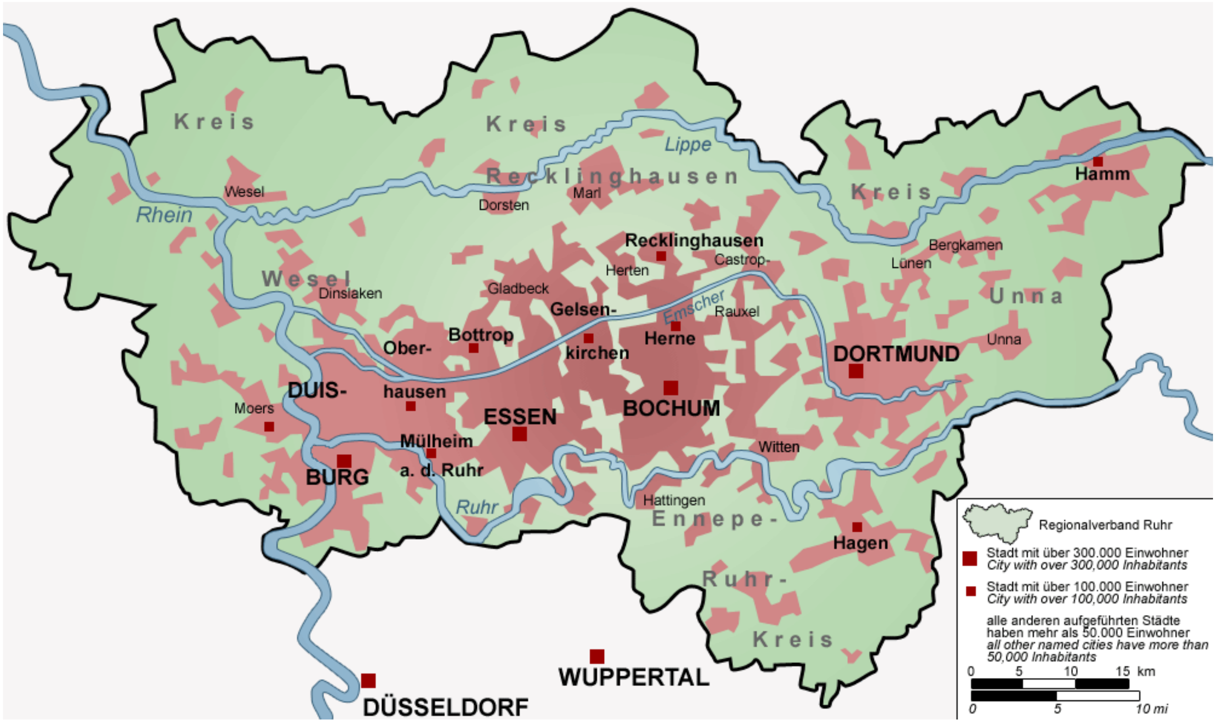

Figure 9-1 Ruhr map mentioning all cities above 50000 inhabitants

(Ruhr area map created by Threedots (Daniel Ullrich), license: CC BY-SA 3.0, https://creativecommons.org/licenses/by-sa/3.0/legalcode; no changes were made to the original picture)

9.1.1.4 Description of RMMs/OCs for workers:

The following RMMs apply to formulation activities with CTPht with the intention to reduce worker exposure:

- **Technical measures**
  - In general **all facilities are permanently technically closed systems** (according to the German Technical Instruction on Air Quality Control, TA Luft). When designing the apparatus and the system, the applicable regulations and guidelines were taken into account. All parts of the apparatus are built according to the state of the art (e.g. for sampling there are dead space-free industrial valves from AZ armatures with zero leakage). All apparatus, pumps, vacuum lines and connected components are designed for vacuum.
  - For sampling PÖ-Mix: sampling takes places at **dedicated sampling stations** in the tank farms. A sample vessel is inserted into this sampling box and the door is closed. Only after that the sample vessel is filled by actuating the sampling valve (dead space-free industrial valves from AZ armatures with zero leakage). When the desired amount of sample has been removed, the sampling armature is closed again. A 5-minute waiting period must be allowed before removing the sampling vessel so that the product can cool down and solidify.

- Automated product loading:
  - Before the automated filling process of PÖ-Mix products at the dedicated loading station for trucks can be started all necessary positions of the security chain must be fulfilled, i.e. position of the loading arm, pressure of the arm, ground cable at the truck connected, emergency unlocked, the truck needs to have a filling level below maximum level. These necessities also apply to the central oil loading station
  - The [redacted] is used **to extract the exhaust gases** of the loading stations EPT and PÖ-Mix via the [redacted] and the vacuum pump V10 into the exhaust air system for exhaust gas combustion.
  - After loading of PÖ-Mix products at the EPT, a dripping time of 200 seconds for the loading arm must be observed. An emptying of filling line on-site happens automatically on the container [redacted].

- **Organisational measures**
  - In general there are detailed provisions for training of employees (e.g. yearly plan of instructions, briefings and trainings; efficacy monitoring of trainings etc. via e.g. feedback questionnaires)
  - Trainings provided in regular intervals are e.g.
    - Proper handling of hazardous substances and compliance with legal regulations and regulations (repetitive training; RÜTGERS Germany contracted medical officer)
    - Instruction in the correct handling of respiratory protective devices and fulfillment of legal regulations and regulations (initial training and repetition; RÜTGERS Germany fire brigade)
    - Proper handling of fire extinguishers and compliance with legal regulations and regulations (repetitive training, RÜTGERS Germany fire brigade)
    - General knowledge of occupational safety (consultancy and/or RÜTGERS Germany SHE responsible)
  - Trainings are performed either by responsible RÜTGERS Germany personnel (e.g. company medical officer) or consultant services with relevant experience.
  - Before working in any facility, which potentially requires wearing of respiratory masks an examination for suitability for mask wearing is performed.
  - Work clothing (e.g. work suit, safety shoes S3) and safety equipment (e.g. safety gloves, helmet with face shield or goggles) is provided by the employer.
  - Work clothes are changed daily or in case of contamination. Working clothes are cleaned by a specialist company (inter alia monitoring of the waste

water), in case of contamination they are disposed of. Otherwise change / care of the PPE is the responsibility of each worker.

- On the site there are locker rooms (use of the black-white clothing change system).
- In maintenance,
  - works are coordinated with the ABF-licence system[2] (see also Table 9-13), but also specific instructions for special cases. **No action is taken without a completed ABF certificate.**
  - For security reasons when opening and closing of the system is required under difficult conditions on-site documentation like "AA-MW-01_Anweisung erschwerte Handhabbarkeit von Arbeitsmitteln beim Öffnen und Schliessen von Systemen" provides further instructions like, that an additional worker has to be in sight in case any situation occurs and is able to alarm first aid personal.
- Accidents:
  - In case of any faults, e.g. when performing works requiring PPE and there is any danger or workers experience difficulty in breathing, specific instructions are in place, i.e. workers need to stop working immediately, have to leave the workplace, drop the respirator and the protective suit and inform the supervisor
  - In case of a necessary emergency emptying of tanks from the EPT (e.g. if there would be a leakage in one tank), there are dedicated operating instructions on how to transfer contents from one tank to another dedicated facility

- **<u>Personal protection measures</u>**

  In general all workers wear:

  - when <u>inside of buildings with no contact to dangerous substances</u>: work suit, safety shoes S3
  - when <u>outside of buildings with no specific task assigned, which could lead to contact with dangerous substances</u>, in addition: helmet, face shield or goggles with side protection
  - when <u>inside of buildings with possible contact to dangerous material</u> (i.e. analysis of sample in dedicated area of control room): all of the mentioned above, but no helmet with face shield, and in addition protective gloves according to glove plan (i.e. disposable nitrile glove under protective leather glove)

[2] ABF certificates include A = working permit („Arbeits-Erlaubnis"), B = passing permit („Befahr-Erlaubnis") and F = fire permit („Feuer-Erlaubnis", works that might throw out sparks)

- o when <u>outside and in case of task assigned within the tank farm, leading to possible contact with dangerous materials</u>, e.g. specific maintenance tasks or cleaning (performed by external specialised contractors) the following additional PPE:
  - Chemical protection suit Microchem 4000 (only maintenance)
  - Respirator with ABEK filter or Respirator with hose
  - Protective gloves according to glove plan or specification via ABF certificate (typically disposable nitrile glove under protective leather glove)
- o But for <u>sampling outside</u> no chemical protection suit is foreseen. The following PPE apply (see also Annex IV – Photo documentation – Sampling, Figure 15-1 to Figure 15-12):
  - work suit
  - Respirator (full mask) with ABEK filter or Respirator with hose
  - Protective gloves according to glove plan or specification via ABF certificate (typically disposable nitrile glove under protective leather glove)

Specificities like wearing time of suits and respiratory protective equipment are provided in specific operating instructions (e.g. for maintenance in "BA-IH-32_Tragezeitbegrenzung_Atemschutzmaske_Chemikalienschutzanzug JBL") and are always according to the national laws (e.g. Protective equipment according to the operating instructions according to §14 GefStoffV for the sampling of liquid carbons).

Work clothes are changed daily or in case of contamination. Working clothes are cleaned by a specialist company (inter alia monitoring of the waste water), in case of contamination they are disposed of. Otherwise change / care of the PPE is the responsibility of each worker.

More details on individual PPE (e.g. standards each item complies with) is provided in Annex VII – Detailed Overview of PPE available including standards complied with.

<u>Considerations on dermal exposure (generally not occurring during normal operations)</u>

In general, as suitable PPE is required and used, no dermal exposure is expected. And as mixtures are hot any contact needs to be avoided to avoid burns. Due to the black colour any contamination of PPEs, like the chemical protective suit or gloves, and possibly skin would be immediately observed. Any incident of contamination is documented in the onsite first-aid centre ("Sani-Stube"). From this documentation it is obvious that from 2014 until 2018 there have been only few situations and thus only a few employees have been shown to be exposed for a short period of time (details are provided in Table 9-12).

Table 9-12: Recordings of treatments in "Sani-Stube" at the RÜTGERS Germany site and specified after incidents with CTPht or AO during the last five years (number of treated workers)

Year	After incident with		Total plant
	CTPht	AO	
2014	0	0	12
2015	1	0	45
2016	3	1	93
2017	1	1	58
2018	3	0	38
total	8	2	246

Incidents reported for CTPht above are mostly skin irritation occurring after working at the bagging station for pelleted neat CTPht and thus are not relevant for this AfA.

The incidents reported in 2017 and 2018 were also reported to be skin irritating effects (in one case corrosive effects), but after contact with formulated products (no further details described).

9.1.1.5 Description of RMMs/OCs for the environment

There is minimal emission of CTPht and AO to air and water, as

a) The facility is designed to be permanently technically tight (e.g. specific design of pipes, tanks and loading stations, all armatures etc.),
b) all tanks are equipped with exhaust pipes on the tops, exhaust air from all tanks is gathered and incinerated on-site,
c) processes are generally water free,
d) rain water, gathered in the tank surrounding tank pits, which might be carrying residual PAH, is gathered and treated on-site via a sand filter and a biological treatment plant (90% efficiency measured as chemical oxygen demand, COD), and
e) wastewater from e.g. cleaning processes performed by specialised external companies are gathered and disposed by the respective contractor at the on-site waste intermediate storage (AZL, see below).

Please note that always total emissions are measured. The contribution from the formulation processes cannot be measured separately. However later on data are presented allowing for the assessment of a proportion of emission generated by this use.

Emissions to water

Processes for manufacturing formulations are essentially without water. Formulating activities are performed in closed systems in a batch procedure without opening and cleaning vessels after emptying. Actually, no cleaning takes place between batches, cleaning with water would anyway be useless, considering the physical nature (semisolid to solid at ambient temperatures) and absent water solubility of the materials.

The only emissions to water, which might occur, are

- Rain water gathering in tank pits (facility wastewater stream: AW3), which contain small particles and contamination from the outside of vessels and tanks (these particles usually not stem from the units where formulation occurs); the level of contamination of these waters is minimal
- Cleaning of loading pipes: this is actually the only cleaning activity taking place in the PÖ-Mix unit. Works are performed by the external maintenance workers from specialised companies. With special cleaning equipment they hose out the pipes with e.g. high-pressure water jet technology, and absorb the emerging wastewater (for details see also WCS6 in section 9.1.8). The wastewater is then brought to the waste intermediate storage (AZL). From waste processing the oil-phase (5%) is fed back into the distillation process, the solid phase (5%) goes to incineration and the rest is further treated via waste water treatment (AW1, biological treatment plant).
- Cleaning of spillage: in case there is any spillage at any of the relevant facilities also specialised companies are providing their service and the wastewater is then brought to the waste intermediate storage (AZL) and treated further from there on as described above (for details on volumes delivered to the AZL and relative proportions of relevant facilities for this AfA, see section 9.1.2 and Table 9-17); spillages due to formulation activities are highly infrequent (included in wastewater volumes of AW1).

The relevant wastewater (for this AfA i.e. stream AW3 and proportion of AW1 coming from cleaning) is treated onsite in a biological treatment plant before being released to Deininghauserbach, which is then called Landwehrbach and is flowing into the Emscher river. The Emscher river is currently flowing openly towards the STP Emschermündung (Dinslaken). Due to its poor water conditions, an extensive reconstruction programme has been initiated. In 2020 RÜTGERS Germany and many other industrial emittents to the Emscher river will have a new waste water distribution system completed. Waste water from the site will be directed in closed underground tubes towards the STP Emschermündung (Dinslaken), which is just located approximately 40 km west of the RÜTGERS Germany site. The Emscher river will be renaturated. Cleaned effluents of the municipal STP will be emitted to the Emscher river, which, after a few kilometres, enters the river Rhine. The assessment of emissions to water is based on this new situation to be realised in 2020 (for further details see 9.1.2).

Liquid port (qualitative):

There are special measures in order to ensure water protection also during barge loading at the liquid port. There are technical measures installed in order to monitor and detect leakage, to avoid overflow, to limit any leakages and for retention. Also the existing, fortified area below the effective range of the loading arm withholds drip leaks. Due to the upturn of the steel frame of the pier it is ensured that drip leaks cannot drain into the harbour basin.

Emission to air

As explained above, all tanks are equipped with exhaust pipes on the tops and also all relevant loading stations are equipped with exhaust air extraction systems. Exhaust air from all tanks and all relevant loading stations (i.e. PÖ-Mix loading station, central oil loading, barge loading facilities and filling nozzle of drum filling station) is collected and incinerated on-site.

Site specific details for different parts of the facility are provided below:

The **tank farm (EPT)** has a vacuum slop system [redacted] with connected drain point, which can also be used to unload tankers. The slop system [redacted] is also used to extract the exhaust gases of the loading stations EPT and PÖ-Mix via the [redacted] and the vacuum pump [redacted] into the exhaust air system for exhaust gas combustion. The [redacted] collects fluid components. Via slop lines relevant tanks, amongst others e.g. PÖ-Mix, are connected to the [redacted] to aspirate liquids. Draining tankers via the drain point is done by means of the vacuum system in [redacted]. The emptying of the [redacted] is realized via the pump [redacted] in the direction of the group input distributor [redacted].

The exhaust gases from the tank groups and the PÖ-Mix are cleaned via a common vapour recovery system and sent to waste gas combustion. In detail, the exhaust gas is extracted via the [redacted] by means of a jet pump and washed. To operate the jet liquid pump, wash oil from the circulation line of [redacted] is moved into the container. At the same time, used wash oil is returned to the circuit. The vapour recovery system of the EPT is rendered inert with nitrogen by means of a regulator system. The ventilation system maintains a pre-set pressure of 5 mbar (g), which is controlled by the PLS of the [redacted] units. If the set pressure falls short, the exhaust flap is opened towards the jet liquid scrubber on the [redacted], so that the washed exhaust gases are passed to the exhaust system. When the set pressure is exceeded, the exhaust flap is closed to [redacted] and nitrogen is added to the vapour recovery system. In addition, the tanks are protected with heated underpressure and overpressure safeguards ("Protegos"). Filling and emptying operations may only be carried out in the EPT when the incineration, waste gas scrubbing and vapour recovery system are operational.

The **Ölbetrieb** plant contains various pumps, filters, pipelines and heat exchangers as well as sampling points in closed systems. If necessary, the devices are equipped with safety fittings (detonation, overpressure, underpressure, overfill protection). In addition to existing fire protection devices such as push button detectors in the adjacent areas powder extinguishers are attached to the entry points. Emergency showers are located at various destinations nearby (i.e. the control room ([redacted]), to the east of the [redacted] plant ([redacted]).

Incineration

The exhaust air streams from the plants of RÜTGERS Germany are collected in five different waste gas streams (exhaust gas network) and removed via the incineration plants (exhaust gas combustion facility, AVS). The calorific value of the exhaust gases is exploited to generate steam.

The exhaust air streams are thermally treated in three combustion systems (AVS 1, AVS 2 and AVS 3). These exhaust gas incinerators and a flue gas desulphurisation unit (REA) are combined to form a composite system, which ensures the combustion of all exhaust air streams.

The exhaust gas combustion plants with heat recovery (AVS1 and AVS 3) are operated in parallel. Both incinerators are equipped with a common denoxification stage (DeNOx) and flue gas desulphurisation unit (REA), which is used to treat both the flue gases of the AVS 1 and the AVS 3. The combustion chamber temperatures are 900°C in both units and the oxygen content in the flue gas is 10%. The AVS 1 is designed for a 1 second dwell time and the AVS 3 for 2 seconds[3].

The AVS 2 - without steam generation and without REA - is used to burn peak quantities, especially when the AVS 1 or the AVS 3 is not available.

The exhaust air stream for the northern area, in which all of the relevant facilities are located is called stream "40-4 (north)". This stream has no connection to AVS 2 and is always headed to AVS 1 and 3. In reality, all exhaust gas streams are subject to qualitative and quantitative fluctuations. The following process data were used as the basis for the design of the systems for the relevant exhaust stream 40-4 (north):

- maximum mass flow = 2137 kg/h;
- caloric value = 0.19 kWh/kg;
- operating temperature approx. 80°C;
- pressure at plant limit 0-30 bar ü;
- standard density 1.28 kg/Nm^3;
- security zone according to German Ordinance on Industrial Safety and Health (BetrSichV) = 0.

The composite system is controlled via the PLS situated in the control room for supply and disposal. Here all essential temperature, pressure and flow parameters of the plants are visualized. Some site specific documentation and certificates containing limit values for emissions and for the flue gas unit are provided in Annex II – Details on exhaust gas combustion facilities.

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). But 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:

[3] The literature usually assumes 1 second sufficient to completely burn PAHs.

- Implementation of mobile PID-devices to observe work tasks like opening pipes
- Site immission measurement concept for the site with gaschromatography stations to detect immissions in µg scale with automated alarm triggering according to incident prevention / mitigation concept
- Continuous measurements of benzene
- Measurements of VOCs e.g. in [redacted] and [redacted] pellet plant.

9.1.1.6 Handling of waste

Delivery, acceptance and transport of hazardous waste is documented and accounted for using the electronic waste detection procedure (eANV).

No waste from/during production occurs as off-spec production is recycled for upgrading. Work up of cleaning water from tank revisions and other maintenance activities as well as cleaning of pipes and possible spillages are described below in section 9.1.2 and Table 9-17.

Samples as well as solid residues from vacuum truck operations or residues from cleaning of the filling nozzles from drum filling station are treated by incineration.

Any product-contaminated waste that might occur and is not incinerated will be handled according to national cycle management act (“Kreislaufwirtschaftsgesetz”, KrWG). Basically, almost all product-contaminated waste is classified as "hazardous waste". In this case, a complicated set of rules is used, in which the individual wastes are analysed and classified. They can then only be disposed of with approved transporters and the disposal companies. Waste type, quantities, waste producers, transporters and disposers can be transparently presented to the monitoring authorities by means of so-called "waste disposal certificates" and accompanying transport accompanying documents. Wastes that have to be disposed of via waste disposal certificates are exemplified in Annex III – Waste disposal notifications.

9.1.1.7 Description of technical improvements achieved and planned

Table 9-13: Plant improvements

Item	Details/Rationale	Status
Improvements implemented and in operation		
Equipment modification	Several modifications with the goal to further improve safe work and reduce leakage into the work area: ▪ overpressure and underpressure protection with inspection flaps ▪ temperature control of container contents ▪ Overfill protection LZA+ (light signalling system) at 95% of the tank volume with shut-off of the filler flap. ▪ Level measurements with shutdown of the agitators at L (low level). ▪ Pressure measurement with shutdown at P (max) (filling flap) and P (min). Everything according to German national law (TA Luft)	Implemented within the last years
Control of technical conditions via measurements of accredited measuring laboratories at regular intervals	E.g. measurements according to TRGS 402 approximately every two years. Results thereof are presented to the responsible national authorities. This ensures functionality of the technical measures to reduce exposure.	In operation
Power outage plan	▪ The loss of electrical energy would affect the following technologies in the facilities relevant for this application: • Measuring and control technology (MSR facilities) • Feed pumps ▪ The power supply of the factory is redundant. If both power supplies fail, all equipment moves in their respective safety position, which converts the entire plant into a lower-energy and therefore safer state. Dangerous effects are thus excluded.	

Item	Details/Rationale	Status
Organisational change - ABF-licence system[4]	ABF-licence introduction leads to lower exposure of maintenance workers, as specific task assignment and description of RMMs and PPEs are now standardised	Modified in 2014, but in place since three decades
Implementation of behavioural safety campaign	Compulsory regular management safety walks	Implemented since three years
Increase of number of safety inspections		Implemented within the last three years
Execution of „STOP-THINK-ACT safely " campaign	DUPONT- licensed system to improve the safety behaviour	Implemented within the last three years
Implementation of safety talks with employees during safety rounds		Implemented within the last three years
Special training for use of breathing masks		Implemented within the last three years
Implementation of mobile PID-devices	to observe work tasks like opening pipes	Implemented within the last three years
Site immission measurement concept for the site with gaschromatography stations	to detect immissions in µg scale with automated alarm triggering according to incident prevention / mitigation concept	Implemented within the last three years

4 The ABF-licence system means that before any maintenance work is performed the maintenance coordinator and the responsible production employee will discuss necessary actions and set a deadline for implementation. Before starting any maintenance work the performing maintenance employee will receive the necessary "ABF certificates" (see also on-site operation procedure AA-IH-05 (checked in regular intervals) and the template working permission form "Arbeitserlaubnis (Formular)"), which are filled from the production department. These are to be fetched by the maintenance engineer before starting work and to be checked for completeness. The production responsible and the maintenance responsible provide all necessary signatures and content in terms of safety precautions, workflows, PPE etc., which are to be followed. No other activities than described on the ABF certificate are carried out. This also applies to activities in the immediate environment. If production desires any further activities a separate ABF certificate is created. No action is taken without a completed ABF certificate.

Item	Details/Rationale	Status
Intended improvements		
Relocation of drum filling station to northern area	IBC filling station currently used for [redacted] + AO mixtures is relocated to the [redacted] unit in the northern part of the site → transfer by railcars between distant locations is avoided	Commissioning planned for Q1 2019
Last minute risk assessment for unusual tasks		Q1 2019
Lock out / tag out		

9.1.2 Environmental contributing scenario 1

9.1.2.1 Conditions of use

Table 9-14: Conditions of use

Amount used, frequency and duration of use (or from service life)
• Annual use amount at site: [redacted] (25 000-400 000) tonnes CTPht/year and [redacted] (10 200-106 000) 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 incinerated on-site.
Conditions and measures related to wastewater treatment
• Formulations are produced without water • On-site treatment of rainwater and cleaning water: yes, biological WWTP; the on-site pre-treated water is then led to an external STP • Discharge rate of on-site WWTP: 604 000 m^3/year (= 0.019 m^3/sec) in 2017 • External biological STP: Standard (removal rate: 69-91%; depending on the individual PAH) • Application of sludge from on-site WWTP on agricultural soil: No • Application of sludge from external STP on agricultural soil: No • Discharge rate of external STP: 1.5-16 m^3/sec (to Emscher River)
Conditions and measures related to external treatment of waste (including article waste)
• Particular considerations on the waste treatment operations: solid waste is collected and incinerated on-site
Other conditions affecting environmental exposure
• Receiving surface water flow rate: 7.88 m^3/sec (based on the calculation as shown below in section 9.1.2.3)

9.1.2.2 Releases

Table 9-15: Local releases to the environment from formulation processes using CTPht and AO

Release	Release rate estimation method	Explanation / Justification
Water	measured	Local release rate to external STP: 5.11 g/day (mean daily release rate for 2017; sum of 9 PAHs relevant for the PBT assessment of CTPht and AO, for individual substances see

Release	Release rate estimation method	Explanation / Justification
		Table 9-19) Explanation / Justification: measured data Emission to surface water from external STP: 1.00 g PAH/day (mean daily release rate for 2017; sum of 9 PAHs relevant for the PBT assessment of CTPht and AO, for individual substances see Table 9-20) Explanation / Justification: modelled data
Air	-	Initial release factor: 0% Final release factor: 0% Local release rate: 0 kg/day Explanation / Justification: complete incineration
Soil	-	Final release factor: 0% Explanation / Justification: no emission to soil

Releases to waste
The amount of waste arising from formulation activities at RÜTGERS Germany is negligible. Only solid waste (e.g. contaminated gloves, sample containers, solid phase resulting from cleaning activities (see Table 9-17) is produced in very small quantities, which is incinerated on-site or 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:

Emission to air

All tanks are equipped with exhaust pipes on the tops and also all relevant loading stations are equipped with exhaust air extraction systems. Exhaust air from all tanks and all relevant loading stations (i.e. PÖ-Mix loading station, central oil loading, barge loading facilities and filling nozzle of drum filling station) is collected and sent to on-site thermal oxidation. Since the exhaust gas is completely incinerated, the emission to air is negligible (incineration at 900°C; 1-2 seconds of gas residence time). Total organic carbon measurement is carried out as a regulatory requirement every three years as a discrete measurement.
Further emissions to air via volatilization from surface waters (or e.g. the collection basins of the on-site treatment 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, 2009a; The Netherlands, 2008).

Emission to water

The whole formulation processes are waterless and no wastewater needs to be considered for this AfA. Only the rainwater gathering in tank pits (see below facility wastewater stream AW3) and cleaning water from the cleaning of loading pipes by an external service provider or from spillage cleaning in respective areas (see below, only part of facility wastewater stream AW1) is relevant for this AfA.

However, PAH measurements are only available for the total effluent of the on-site biological WWTP.

In general there are **four wastewater streams (AW)** in the facility leading to the on-site WWTP:

- AW1: coming from production (highly contaminated) plus waste water from cleaning activities (moderately contaminated) (see Table 9-16 and Table 9-17 for amount relevant for the assessment in this AfA),
- AW2: e.g. from cooling systems (practically not contaminated, not relevant for this AfA)
- AW3: rainwater coming from tank pits (low contamination; relevant for the assessment in this AfA),
- AW4: rainwater from sewerage (low contamination due to PAHs in soil, not relevant for this AfA)

There are data (4 per year) for the individual wastewater streams, which allow assessing the relative contributions of each stream. Measurements for the AW1 current are on average around 15 000 µg PAH/L, whereby the values vary between 500 and 280 000 µg PAH/L. There are fewer data available for the AW3 of the northern part of the plant (1 per year). Here the mean value is 400 µg PAH/L. The values vary between 16 and 1 200 µg PAH/L. Based on assumptions and data, the following balance of PAH loads can be presented.

Table 9-16: Overview on waste water streams of the facility (based on data from year 2015 to 2017) directed to the on-site WWTP

		AW1	AW2	AW3	AW4	Sum incoming
Amount of water	m^3/a	69 000	184 000	32 000	331 000	616 000
PAH concentration	µg/L	15 000	15	400	300	1 850
PAH emission (release of total PAH to on-site biological WWTP)	kg/a	1 035	2.8	12.8	99.3	1 140
Percentage assumed to be related to formulation activities		2.9%	0%	100%	0%	3.8%
Relevant for this AfA	**kg/a**	**30**	**-**	**13**	**-**	**43**

The amount relevant for this AfA from wastewater stream 1 (AW1) results from volumes from cleaning activities (performed via vacuum trucks) in areas were formulation occurs (i.e. 2 000 m^3/a, for details see Table 9-17 below) relative to the total volume of the AW1

(69 000 m^3), i.e. 2.9%. Note that this assessment is conservative as we assume that waste water from vacuum truck services is polluted the same way as waste water coming from production, which is typically not the case. In addition, not all of the volumes coming from the relevant facilities are necessarily related to formulation processes, thus adding another layer of conservatism to this assessment.

Adding up the relevant part of AW1 plus the load from AW3 the total load considered relevant for this assessment yields 43 kg/a, which equals around 3.8% of the total PAH load to the on-site biological WWTP. **For the further assessment 5% will be considered.**

This assumption is not affected with higher amounts of CTPht formulations being produced in the future, as the calculated fraction of AW1 already accounts for all cleaning water coming from Ölbetrieb and PÖ-mix (see below for details).

Details on wastewater from cleaning/maintenance operations

Contaminated waste water from tank revisions and maintenance activities such as the cleaning of loading arms is taken up by “chemistry vacuum trucks”. Around 8 000 to 9 000 tonnes of suspensions are worked up via this system at the RÜTGERS Germany site per year, the larger part originating from tank cleanups and other activities not related to formulation activities (for details see Table 9-17). As a first step of the clean-up sedimentation is allowed to take place in work-up tanks. From the subsequent decanter centrifuge the oil-phase (5%) is fed back into the tar distillation, the solid phase (5%) goes to the on-site incineration; the remaining stream goes to wastewater stream 1 (AW1), which is then directed towards the on-site biological WWTP.

The total volume of waste water coming from Ölbetrieb (1 213 m^3 wastewater/a) and PÖ-mix (481 m^3 wastewater/a) is conservatively assumed to be related to formulation activities and is included in the assessment. This amounts to 2 000 m³ or 2.9% (out of ~69 000 m^3) of wastewater stream AW1.

Table 9-17: Wastewater from chemistry vacuum trucks fed into waste intermediate storage (AZL)

	2015 [m³] (%)	**2016** [m³] (%)	**2017** [m³] (%)	**Mean** [m³] (%)
Sum incoming at AZL	8 964 (100)	9 941 (100)	9 934 (100)	9 613 (100)
Water phase	7 583 (85)	9 273 (93)	9 219 (93)	8 692 (90)
Oil phase	802 (9)	466 (5)	380 (4)	549 (6)
Solid phase	579 (6)	202 (2)	335 (3)	372 (4)
Detail – Sum incoming at AZL from „Ölbetrieb“	1 255 (14)	1 094 (11)	1 291 (13)	1 213 (13)
Water phase (proportionally)	1 062	1 020	1 198	1 093
Oil phase (proportionally)	112	51	49	71
Solid phase (proportionally)	81	22	44	49
Detail – Sum incoming at AZL from EPT (PÖ-Mix + [redacted] unit)	No detailed data available. However approximation by on-site waste responsible person was 2-5% → 5% = 481 m³ will be used for the further assessment			
Sum used for further assessment	1 213 + 481 ≈ **2 000 m³**			

<u>Emission to the external STP "Emschermündung"</u>

As mentioned the relevant wastewater stream AW3 (rainwater from tank pits) and also AW1 (relevant proportion of water from cleaning/maintenance operations) are treated on-site in the biological WWTP. The effluent of the on-site biological WWTP is measured at least once per month in the years 2015-2017 (21-26 measurements per year in 2015-2017; monthly measurement required according to the release permit) for concentrations of individual PAHs. In 2018, the PAH concentrations were only measured between August and November (6 measurements). The individual measurements are provided in Annex IX – PAH drainage after biological treatment plant. Yearly means were calculated from the individual measurements and multiplied with the wastewater discharge volumes per year in order to obtain the emissions of the individual PAHs.

The concentrations and the emissions 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) are provided together with the wastewater discharge volumes in Table 9-18.

Table 9-18: Yearly mean PAH concentrations, discharge volumes and emission values for the years 2015-2018

	2015			2016			2017			2018		
PAHs	Conc. [µg/L] [a]	Total emission [g/y]	Total emission [g/d]	Conc. [µg/L] [a]	Total emission [g/y]	Total emission [g/d]	Conc. [µg/L] [a]	Total emission [g/y]	Total emission [g/d]	Conc. [µg/L] [a]	Total emission [g/y]	Total emission [g/d]
Anthracene	0.57	365.7	1.0	1.86	1 124.8	3.1	2.55	1 537.18	4.21	2.07	1 240.0	3.4
Phenanthrene	1.61	1 031.3	2.8	12.83	7 759.4	21.3	18.70	11 293.43	30.94	15.20	9 120.0	25.0
Fluoranthene	1.80	1 149.9	3.2	26.69	16 146.8	44.2	23.76	14 349.12	39.31	12.85	7 710.0	21.1
Pyrene	1.31	841.4	2.3	13.25	8 016.1	22.0	11.13	6 719.50	18.41	10.53	6 320.0	17.3
Benz[a]anthracene	0.21	131.7	0.4	0.68	413.3	1.1	1.48	892.27	2.44	0.82	490.0	1.3
Chrysene	0.29	187.4	0.5	1.18	715.8	2.0	1.49	897.49	2.46	1.28	770.0	2.1
Benzo[a]pyrene	0.42	265.8	0.7	1.07	648.3	1.8	1.43	865.09	2.37	2.50	1 500.0	4.1
Benzo[b]fluoranthene [b]	0.50	317.0	0.9	1.64	991.7	2.7	1.85	1 116.30	3.06	3.60	2 160.0	5.9
Benzo[k]fluoranthene	0.22	140.2	0.4	0.64	389.1	1.1	0.75	454.10	1.24	1.12	670.0	1.8
Benzo[ghi]perylene	0.39	247.8	0.7	0.51	309.5	0.8	0.52	312.71	0.86	1.15	690.0	1.9
Sum 9 PAHs relevant for PBT assessment		4 361.14	11.95		35 522.90	97.32		37 320.89	102.25		28 510.00	78.11
Sum 4 EFSA PAHs relevant for HvE assessment		901.79	2.47		2 769.04	7.59		3 771.16	10.33		4 920.00	13.48
Total volume [m^3/year]	640 000			605 000			604 000			600 000		
Total volume [m^3/day]	1 753			1 658			1 655			1 644		

Unrounded values used for calculation.

[a] PAHs measured in wastewater at the RÜTGERS Germany GmbH laboratory according to DIN EN ISO 17993 with HPLC (fluorescence detection) after liquid-liquid extraction (limit of detection: 0.1µg/L or 0.1ppb).

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

From the numbers shown in the table above, a conservative set was selected for the environmental assessment. In 2018, the PAH concentrations were only measured between August and November and the yearly mean concentrations were calculated based on these 6 individual measurements. Thus, the concentrations and emission values are not considered representative when compared with the years 2015 to 2017, where PAH concentrations were measured throughout the years and yearly means are calculated from at least 21 individual values per year.

The emission sum for the 9 PAHs relevant for the environmental PBT assessment (all PAHs shown in the table except benzo[b]fluoranthene) and also the sum of the 4 EFSA PAHs (benz[a]anthracene, chrysene, benzo[a]pyrene and benzo[b]fluoranthene) relevant for the assessment for humans via the environment (HvE) was highest in 2017 (only the sum of the 4 EFSA PAHs is by a factor of 1.3 slightly higher in 2018 than in 2017, but the values for 2018 are not considered representative, as described above). These high emission values in 2017 can be explained by repair works, which were carried out during this year and which affected the stable functioning of the biological on-site WWTP.

Nevertheless, the emission values from 2017 were used as input data for EUSES modelling in order to assess the environmental exposure conservatively.

Since **only 5% of the total PAH emissions** are relevant for this AfA (as described above, Table 9-16), the total PAH emissions and the 5%-fraction thereof are presented in Table 9-19.

Table 9-19: PAH release rates for on-site pre-treated wastewater from the biological WWTP at RÜTGERS Germany to the external STP in 2017

PAHs	Release rate [g/year]	Release rate [g/day]	5% of total emission [g/y]	5% of total emission [g/d]
Anthracene	1 537.18	4.21	76.86	0.21
Phenanthrene	11 293.43	30.94	564.67	1.55
Fluoranthene	14 349.12	39.31	717.46	1.97
Pyrene	6 719.50	18.41	335.98	0.92
Benz[a]anthracene	892.27	2.44	44.61	0.12
Chrysene	897.49	2.46	44.87	0.12
Benzo[a]pyrene	865.09	2.37	43.25	0.12
Benzo[b]fluoranthene *	1 116.30	3.06	55.82	0.15
Benzo[k]fluoranthene	454.10	1.24	22.70	0.06
Benzo[ghi]perylene	312.71	0.86	15.64	0.04
Sum 9 PAHs relevant for PBT assessment in CTPht	37 320.89	102.25	1 866.04	5.11

Unrounded values used for calculation.
* Not PBT; environmental modelling performed as substance is required for calculating the sum of 4 EFSA PAHs for the assessment of HvE

The pre-treated wastewater is piped to an external STP, which is adapted to the treatment of industrial wastewater. Currently, the water is released to the Deininghauserbach, which is later called Landwehrbach and is flowing into the Emscher River (approximately 5 km). The Emscher River receives large quantities of industrial wastewater from numerous companies being located alongside the river. Downstream of the Emscher River, in approximately 35 km distance, the external STP "Emschermündung" is situated, which receives the total water volume of the Emscher River for treatment (see Figure 9-2). After the external STP, in approximately 5-6 km distance, the Emscher River flows via a fall into the Rhine River (see Figure 9-3).

Figure 9-2: **Location of the wastewater discharge point of RÜTGERS Germany, the external STP "Emschermündung" and the gauging station "Oberhausen Königsstraße" along the Emscher River[5]**

[5] https://www.google.com/maps

Figure 9-3: Location of the external STP "Emschermündung" approximately 6-7 km upstream of the opening of the Emscher River to the Rhine River[6]

By beginning of 2020, the situation will be different from now. The industrial wastewater from RÜTGERS Germany and other companies will then be led through a closed, underground channel ("Abwasserkanal Emscher", AKE) to the external STP. Therefore, the channel is currently built and the external STP is modified in order to deal with lower, but more concentrated wastewater volumes in the future (information provided on the website of the Emschergenossenschaft Lippeverband (EGLV)[7]. The Emscher River will then bypass the external STP and only receive the cleaned water released from the external STP. After being recultivated, the Emscher River will then meander to the estuary and naturally flow into the Rhine River (information provided on the website of the Emschergenossenschaft Lippeverband, EGLV[8]).

Since the situation from beginning of 2020 onwards is the relevant scenario for this AfA, the environmental assessment is based on the future conditions. The total wastewater from RÜTGERS Germany will then be led through the closed channel underground to the external STP "Emschermündung", which will have a total discharge flow of 1.5 to 16 m^3/sec. (information provided by the EGLV during oral communication on 10th December 2018). The total volume of the Emscher River downstream of the external STP can be expected to be similar to its volume at the present situation. There is a mean low stream flow (MLQ) of 9.38 m^3/sec provided for the gauging station "Oberhausen Königsstraße" (information according

[6] www.google.com/maps
[7] Emschergenossenschaft Lippeverband (EGLV); news item from 4th April 2017 http://www.eglv.de/medien/presseinformationen/pressemitteilung/?tx_ttnews[tt_news]=762&cHash=76790c72f9788c8bc2ff6bdf9430374c#; accessed on 12th December 2018
[8] Emschergenossenschaft Lippeverband (EGLV); https://www.eglv.de/fileadmin/user_upload/pdf/BI_EG_Emschermuendung_V2.pdf; accessed on 12th December 2018

to https://www.flussgebiete.nrw.de[9]), approximately 4 km upstream of the external STP (see Figure 9-2; changes in the river flow over 4 km distance are expected to be negligible).

However, at the discharge point, the expected flow rate of the Emscher River under the new conditions is the current flow rate minus the discharge flow of the new external STP (since all wastewater is led to the external STP via the underground channel and not through the Emscher River). Accordingly, by calculating with a discharge flow of 1.5 m^3/sec of the new STP (as a conservative assumption for dilution of wastewater discharges of RÜTGERS Germany in the external STP), it is expected that the Emscher River will have an MLQ of only 7.88 m^3/sec (9.38 m^3/sec -1.5 m^3/sec = 7.88 m^3/sec) at the discharge point.

Approach to EUSES modelling

EUSES modelling was performed for the external STP, using the releases to this STP from the on-site WWTP shown in Table 9-19.

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 *fractions of tonnage released to air, surface water and industrial/agricultural soil* were set to 0 (according to Table 9-15).
- The local *fraction of tonnage released to wastewater* was calculated by dividing the water emission from formulations (5% of total wastewater from the plant; e.g. [g/day]; as provided above in Table 9-19) 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:
    - 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 Tabel 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 the on-site WWTP are based on measured data.
- The *number of emission days per year* is 365
- The local distribution of sludge from the STP to soil or grassland was set to 0 in the EUSES default setting (*defaults -> local distribution -> soil -> dry sludge application*

[9] www.flussgebiete.nrw.de/system/files/atoms/files/emr_bestandsaufnahme_2004_emscher.pdf

rate on agricultural soil/grassland = 0), since no sludge produced in the on-site WWTP at RÜTGERS Germany or at the external STP "Emschermündung" is applied to soil or grassland (the sludge from the on-site WWTP is delivered to the external STP in Bottrop (also belongs to Emschergenossenschaft Lippeverband, EGLV), here the sludge is mixed with others and incinerated).

- 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.* Then, 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 direct release into surface water is present in the local scenario, the release fractions on the regional scale were adjusted accordingly: 100% (instead of 80%) as *total regional emission to wastewater* and 0% (instead of 20%) as *total regional emission to surface water*. Then the regional distribution of sludge to soil was eliminated by setting the *indirect emission to agricultural soil* in the *regional STP* to 0. 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.

- A discharge flow of 1.5 m^3 per second (= 129 600 m^3 per day; 50 457 600 m^3 per year) was assumed for the external STP "Emschermündung" from beginning of 2020 onwards (as a worst case estimate, based on the information that the reconstructed WWTP will have discharge rates of 1.5-16 m^3/sec, as described above)

- The flow rate of the Emscher River will be reduced by the discharge flow of the new external STP from beginning of 2020 onwards. Accordingly, an MNQ of only 7.88 m^3/sec is expected for the Emscher River at the release point, assuming the minimal discharge flow of 1.5 m^3/sec (as described and calculated above). Based on this, a dilution factor of 6.25 for cleaned wastewater from the external STP discharged into the Emscher River ((7.88 m^3/sec + 1.5 m^3/sec) / 1.5 m^3/sec = 6.25) is calculated.

- 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 German food consumption from the Max Rubner-Institute ("Nationale Verzehrsstudie II") (MRI, 2008), 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 German population. The EUSES defaults were compared with the numbers from the survey (in cases where an EUSES food category consists of more than one group considered in the survey, the sum of all groups was calculated). The composition and consumed amounts of these five food categories are provided in Annex X – German food consumption, "Nationale

Verzehrsstudie II". 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 XI – EUSES Protocols.

EUSES output data

Water, sediment and soil

The following Table 9-20 gives the result of the emission modelling with EUSES for the distribution of individual PAHs to various compartments. Note that the emissions to water are further distributed to the sediment.

As zero emission to air is assumed at the site (incineration of exhaust air) emission to air occurs only from the external STP.

Table 9-20: PAH emissions from the external STP to various compartments

PAHs	Release rate to external STP [g/year]	Emission to surface water from external STP [g/year]	Emission to sludge from external STP [g/year]	Emission to air from external STP [g/year]
Anthracene	76.83	19.75	56.49	0.58
Phenanthrene	564.68	167.71	392.45	4.52
Fluoranthene	717.25	102.60	614.14	0.51
Pyrene	335.78	60.48	274.83	0.48
Benz[a]anthracene	44.62	4.15	40.46	0.00
Chrysene	44.90	4.33	40.57	0.00
Benzo[a]pyrene	43.25	3.81	39.45	0.00
Benzo[b]fluoranthene*	55.82	4.91	50.90	0.00
Benzo[k]fluoranthene	22.71	2.00	20.71	0.00
Benzo[ghi]perylene	15.64	1.35	14.29	0.00
Sum of 9 PAHs relevant for the PBT assessment	1 865.67	366.18	1 493.38	6.10

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

The Predicted local Environmental Concentrations (local PECs), which were obtained from EUSES modelling for diverse compartments, are shown in Table 9-21 and are compared with the respective Predicted No Effect Concentrations (PNECs), taken from the Annex XV Transitional Dossier.

Table 9-21: Local PECs (calculated by EUSES) for different 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	6.42E-08	1.90E-04	8.02E-09	1.00E-04	1.40E-01	1.26E-01
Phenanthrene	5.52E-07	1.27E-03	6.20E-08	1.30E-03	5.00E+00	1.80E+00
Fluoranthene	3.05E-07	2.98E-03	1.89E-08	1.00E-05	9.60E-01	1.50E+00
Pyrene	1.89E-07	1.11E-03	1.04E-08	2.30E-05	2.80E+00	1.00E+00
Benz[a]anthracene	8.04E-09	4.03E-04	1.55E-09	1.20E-05	6.01E-01	7.90E-02
Chrysene	9.22E-09	3.67E-04	9.14E-10	7.00E-05	2.79E+00	5.57E-01
Benzo[a]pyrene	5.73E-09	4.77E-04	1.17E-09	2.20E-05	1.83E+00	5.30E-02
Benzo[k]fluoranthene	3.10E-09	2.46E-04	2.71E-10	1.70E-05	1.35E+00	2.70E-01
Benzo[ghi]perylene	1.81E-09	1.85E-04	9.30E-11	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 9-22).

Table 9-22: Local RCRs for diverse compartments as calculated by EUSES

	RCR fresh water	RCR fresh sediment	RCR soil
Anthracene	6.42E-04	6.77E-04	6.37E-08
Phenanthrene	4.24E-04	1.27E-04	3.45E-08
Fluoranthene	3.05E-02	1.55E-03	1.26E-08
Pyrene	8.21E-03	1.99E-04	1.04E-08
Benz[a]anthracene	6.70E-04	6.70E-03 *	1.97E-08
Chrysene	1.32E-04	1.32E-03 *	1.64E-08 *
Benzo[a]pyrene	2.61E-04	2.61E-03 *	2.21E-08
Benzo[k]fluoranthene	1.82E-04	1.82E-03 *	1.00E-08 *
Benzo[ghi]perylene	2.21E-04	2.21E-03 *	5.56E-09 *

* 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 (EC, 2008), available for anthracene, fluoranthene and benzo[a]pyrene shows that the water emissions from RÜTGERS Germany have a negligible impact on the environment. The calculated $PEC_{freshwater, bulk}$ values of the individual PAHs are between two and four orders of magnitude lower than the Environmental Quality Standard for inland surface waters (Table 9-23). Accordingly, the predicted environmental PAH concentrations resulting from RÜTGERS Germany´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 9-23: Comparison of PEC values for bulk freshwater 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	6.88E-08	1.00E-04	6.88E-04
Phenanthrene	5.83E-07	-	
Fluoranthene	3.78E-07	6.30E-06	5.99E-02
Pyrene	2.16E-07	-	
Benz[a]anthracene	1.78E-08	-	
Chrysene	1.81E-08	-	
Benzo[a]pyrene	1.73E-08	1.70E-07	1.02E-01
Benzo[k]fluoranthene	9.09E-09	[d]	
Benzo[ghi]perylene	6.32E-09	[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 (EC, 2008)
[c] Inland surface waters encompass rivers and lakes and related artificial or heavily modified water bodies (EC, 2008)
[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 (EC, 2008)

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 Emscher River close to the external STP "Emschermündung".

PAH measurements for two sampling sites are accessible via elwasweb.nrw.de[10]; at measurement station ID 50600, which is located a few meters upstream of the discharge point of the external STP "Emschermündung" (exact location of the discharge point not indicated), and at measurement station ID 005009, situated approximately 5 km downstream of the discharge point of the external STP (see Figure 9-4).

[10] https://www.elwasweb.nrw.de; accessed on 7th January 2019

Figure 9-4: Measurement stations close to the STP "Emschermündung"

The PAH concentrations measured in surface water upstream of the external STP, at station ID 506000 (most recent data available are from 2016) and the concentrations measured downstream, at station ID 005009 (most recent data available are from 2016-2018) are compared with each other and with the calculated local PEC in surface water. As shown in Table 9-24, the concentrations measured for each individual PAH at the station (ID 005009) downstream of the external STP remained relatively constant during the three years 2016-2018. These concentrations are by a factor of 2.5-24 lower than the concentrations measured in 2016 at the station (ID 506000) upstream of the external STP in the Emscher River.

The PECs in freshwater (calculated based on emission data from 2017) of the smaller (3-4-ringed) PAHS are between two and four and of the larger PAHs (5-6-ringed) five orders of magnitude lower than the concentrations measured upstream of the external STP(in 2016-2018).

When compared to surface water concentrations measured downstream of the external STP, the PECs in freshwater of the smaller (3-4-ringed) PAHs are between one and three and of the larger PAHs (5-6-ringed) six orders of magnitude lower than the concentrations measured at station ID 005009 (in 2016).

Overall, these data indicate a low environmental impact of the water emissions from RÜTGERS Germany on environmental PAH concentrations in the Emscher River. Based on the measured data at station ID 005009 it is obvious that RÜTGERS Germany is not the only relevant PAH source, since the elevated PAH concentrations in surface water cannot be caused by the water effluents form RÜTGERS Germany alone, even if not only the 5% related to formulation, but the total releases are considered. In addition the assessment of water emission from RÜTGERS Germany was performed conservatively, as the highest emission values from 2017 were used and also the maximum potential tonnages of AO and CTPht for CBO production in Ölbetrieb were considered to contribute to the emission. In reality, if high amounts of AO are used then the required CTPht amount will be lower and vice versa.

Table 9-24: Comparison of PAH concentrations measured upstream (measurement station ID 506000) and downstream (measurement station ID 005009) of the external STP in the Emscher River with PEC freshwater values

	Measurement station ID 506000 (upstream) [a]	**Measurement station ID 005009 (downstream) [b]**			
	Conc. in surface water [µg/L]	Conc. in surface water [µg/L]			Calculated PEC freshwater [µg/L]
Year	2016	2016	2017	2018	
Anthracene	4.93E-02	8.67E-03	5.00E-03	5.00E-03	6.42E-05
Phenanthrene	3.65E-01	4.06E-02	2.05E-02	1.55E-02	5.52E-04
Fluoranthene	1.22E-01	3.63E-02	1.18E-02	1.18E-02	3.05E-04
Pyrene	7.25E-02	2.10E-02	7.09E-03	6.82E-03	1.89E-04
Benz[a]anthracene	3.03E-02	1.23E-02	5.00E-03	5.00E-03	8.04E-06
Chrysene	6.70E-02	1.13E-02	5.00E-03	5.00E-03	9.22E-06
Benzo[a]pyrene	2.10E+01	1.90E+00	2.84E+00	3.36E+00	5.73E-06
Benzo[k]fluoranthene	1.62E+01	2.19E+00	1.45E+00	1.50E+00	3.10E-06
Benzo[ghi]perylene	1.62E+01	1.72E+00	2.63E+00	2.94E+00	1.81E-06

[a] Measured at station ID 506000, EEP14, E31, T11, ST-BR.OH KA EMSCHERM, Emscher; value provided as mean of 4 individual measurements per year.

[b] Measured at station ID 005009, EMR 0-3, Emscher-Mündung , Emscher; value provided as mean of 10-15 individual measurements per year (approx. 1 x per month).

Air

Since all exhaust gases from formulation activities are incinerated (900 °C; 1-2 seconds of gas residence time), no relevant emissions to air from these activities occur at the site (a low extent of volatilisation to air from the on-site WWTP, similar to what has been calculated for the external STP "Emschermündung", can be assumed, see below; that this amount is negligible is confirmed by air measurements close to the production site, see below, measurement point Wartburgstraße).

The predicted environmental concentrations of PAHs in the atmospheric compartment (PEC air) from EUSES modelling (Table 9-25) result from volatilization of PAHs in the external STP. According to the estimated PAH distribution in the STP (as shown in Table 4-6), the fraction released to air decreases with increasing molecular weight, except for anthracene, phenanthrene, fluoranthene and pyrene, where the volatilization of phenanthrene is > pyrene > fluoranthene > anthracene > all other indicator PAHs. With volatilization playing a higher role for these four smaller PAHs, the local PEC_{air} values are three orders of magnitude higher than the regional PEC_{air} values, while the difference between local and regional PECs is in most cases smaller (two to three orders magnitude) for the larger PAHs.

Table 9-25: Local and regional PECs for the atmospheric compartment obtained from EUSES modelling

PAH	Annual average local PEC in air (total) [ng/m^3]	Regional PEC in air (total) [ng/m^3]
Anthracene	4.44E-04	1.34E-07
Phenanthrene	3.46E-03	3.07E-06
Fluoranthene	3.88E-04	7.58E-07
Pyrene	3.65E-04	5.65E-07
Benz[a]anthracene	3.67E-06	1.49E-09
Chrysene	4.58E-07	1.15E-09
Benzo[a]pyrene	1.21E-07	1.08E-09
Benzo[k]fluoranthene	8.37E-08	1.70E-10
Benzo[ghi]perylene	2.82E-08	5.24E-11

Since no PNECs or Environmental Quality Standards are available for the atmospheric compartment, the PECair values are compared with public data for benzo[a]pyrene concentrations measured at survey stations close to the external STP. According to the European Environment Agency (EEA), one measurement station (DENW034; Latitude: 51.524022, Longitude: 6.748402) is located approximately 2 km southwest of the external STP (see Figure 9-5).

Figure 9-5: Location of air measurement station DENW034

At this station, yearly measurements of benzo[a]pyrene in particulate matter with an aerodynamic diameter smaller than 10 µm (PM_{10}) are available for the years 2014-2017. The measured concentrations are provided as yearly mean weighted averages in Table 9-26. The concentrations of benzo[a]pyrene in PM_{10} measured at this station are six orders of magnitude higher than the local and eight orders of magnitude higher than the regional PEC_{air} value calculated for benzo[a]pyrene (from Table 9-25). Accordingly, the air concentration of benzo[a]pyrene (PM_{10}) measured close to the external STP is much higher than the benzo[a]pyrene air concentrations predicted for RÜTGERS Germany and they are unlikely to be affected by emissions coming from wastewater from formulation activities at the plant. Furthermore, since the measurement station is located south-east of the external STP, it can be assumed to be not positioned in wind direction of the external STP (with west wind being the prevalent wind direction in Europe) and, thus, the measured values are assumed to represent background benzo[a]pyrene concentrations in air.

Table 9-26: Air concentrations of benzo[a]pyrene in PM10 measured at station ID DENW034 (2014-2017), provided as yearly mean weighted averages

Year	Benzo[a]pyrene in PM_{10} (aerosol) [ng/m^3]
2014	0.22
2015	0.18
2016	0.32
2017	0.24

In addition to air measurements from the station near the external STP, air emission data are also available from a measurement station positioned very close to the site of RÜTGERS Germany. At the sample site Castrop-Rauxel Wartburgstraße (sampling station DENW264), which is just located outside the north east gates of the plant (see Figure 9-6). As the wind is coming from west / southwest any relevant emission from the RÜTGERS Germany side would be detected at this measurement station.

In a detailed report from RÜTGERS Germany, annual daily mean and maximum concentrations of benzo[a]pyrene (PM_{10}) are reported as 0.33 ng/m³ and 4.1 ng/m³, respectively (n = 160; testing performed between 20.1.2009 and 24.11.2009). For the same year annual daily mean and maximum concentrations of 0.28 ng/m³ and 2.67 ng/m³, respectively, are provided for this measurement station in the European Air quality database (via the Information Platform for Chemical Monitoring (EC, 2019); n = 154).

Figure 9-6: Exact localisation of the sample site Castrop-Rauxel Wartburgstraße (Code: DENW264)[11]

Moreover, data on benzo[a]pyrene exposure can also be seen in the Air Quality e-Reporting (AQ e-Reporting) provided by European Environment Agency (EEA). For Germany for the year 2015 background median air concentrations of benzo[a]pyrene in PM_{10} are reported to be 0.28 ng/m³ (with minimum value of 0.02 ng/m³ and a maximum value of 1.34 ng/m³) (EEA, 2017)[12]. According to this source ambient air concentrations of BaP are high mostly as a result of emissions from the domestic combustion of coal and wood.

The basic data for the year 2015 from the EEA report above can also be accessed and are evaluated according to their regions in the Table 9-27 below.

Table 9-27: Air concentration of benzo[a]pyrene in PM_{10} measured in diverse regions of Germany (2015)

EEA 2015			
Station area	Mean [ng/m³]	Min [ng/m³]	Max [ng/m³]
rural	0.22	0.01	2.37

[11] SOURCE: https://ipchem.jrc.ec.europa.eu/RDSIdiscovery/ipchem/index.html# databaseConsole/AIRBASE/benzo(a)pyrene%20in%20pm10/50-32-8/DEU/none

[12] European Environment Agency (EEA): https://www.eea.europa.eu/data-and-maps/daviz/attainment-situation-for-annual-mean-1, accessed on 14th November 2018

suburban	0.33	0.07	0.89
urban	0.31	0.06	2.49
all	0.29	0.01	2.49
Sub-urban + urban	0.32	0.06	2.49

Source: European Environment Agency [13]; file: ***Air pollutant concentrations 2015 (compared to EU values)***

Moreover, a summary of air concentrations of benzo[a]pyrene in PM_{10} in Germany for 2016, which were most recently published by the European Environment Agency (EEA), are shown in Table 9-28.

Table 9-28: Air concentration of benzo[a]pyrene in PM_{10} measured in diverse regions of Germany (2016)

EEA 2016			
Station area	Mean [ng/m³]	Min [ng/m³]	Max [ng/m³]
rural	0.25	0.02	1.23
suburban	0.39	0.10	1.20
urban	0.38	0.11	1.68
all	0.36	0.02	1.68
Sub-urban + urban	0.38	0.10	1.68

Source: European Environment Agency [14]; file: ***Air pollutant concentrations 2016 (compared to EU values)***

These German background concentrations (Table 9-27 and Table 9-28) of benzo[a]pyrene in PM_{10} are in the same order of magnitude as the reported concentrations measured at the stations DENW264 (located adjacent to the industrial site) and DENW034 (close to the external STP). All measured mean concentrations are in the range between 0.18-0.39 ng/m³.

EUSES calculations predict that the volatilisation of PAHs from the STP lead to undetectable contributions to the air concentrations orders of magnitude lower than background. Therefore, we conclude that there is no significant emission from the site and the wastewaters from the external STP.

<u>Summary – Exposure for the environment</u>

The environmental concentrations conservatively 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

[13] European Environment Agency (EEA); https://www.eea.europa.eu/data-and-maps/data/air-pollutant-concentrations-at-station; accessed on 14th November 2018
[14] European Environment Agency (EEA); https://www.eea.europa.eu/data-and-maps/data/air-pollutant-concentrations-at-station; accessed on 05th February 2019

environmental impact coming from the water and air emissions from formulation activities with CTPht and AO at RÜTGERS Germany is negligible.

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 9-20), AO contributes most of the amount of anthracene (96%) and phenanthrene (95%), two thirds of the amount of fluoranthene (65%) and half of the amount of pyrene (49%), as shown in Table 9-29. The other PAHs are not contained in AO in relevant amounts.

Table 9-29: 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] (25 000-400 000)				
Tonnage AO				[redacted] (10 200-106 000)		
Anthracene	0.057	[redacted]	6.1	[redacted]	3.7	96.3
Phenanthrene	0.302	[redacted]	25.9	[redacted]	4.6	95.4
Fluoranthene	0.835	[redacted]	6.4	[redacted]	35.3	64.7
Pyrene	0.726	[redacted]	2.8	[redacted]	51.5	48.5
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 used for calculation.
[a] According to the European Composite Sample for CTPht (as shown in Table 1-3).
[b] According to the European Composite Sample for AO (as shown in Table 1-4).
[c] tpa = tonnes per annum

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 instead of the EUSES defaults (as described in section 9.1.2.3).

The results of EUSES exposure modelling of humans to PAHs via the environment 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 9-30 on a local and in Table 9-31 on a regional scale.

Table 9-30: 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]	1.35E-03	2.10E-02	9.98E-02	1.05E-03					
	Total daily intake oral (PEC_{oral}) for sum PAH4 EFSA [ng/kg/d]					1.23E-01	2.06E-06			**2.54E-07**
Inhalation general population	Annual average local PEC in air (total) [ng/m^3]	1.21E-07						lung	3.00E-05	**3.63E-12**
								bladder	2.10E-05	**2.54E-12**
								total (lung & bladder)		**6.17E-12**
Workers onsite (not involved in formulation activities)	Annual average local PEC in air (total) [ng/m^3]	1.21E-07						lung	5.60E-06	**6.78E-13**
								bladder	4.00E-06	**4.84E-13**
								total (lung & bladder)		**1.16E-12**

Table 9-31: 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/m³ (excess lifetime cancer risk)		ELCR
Oral general population	Total daily intake oral (PEC_{oral}) for individual PAHs [ng/kg/d]	4.67E-06	8.38E-05	2.95E-04	3.48E-06					
	Total daily intake oral (PEC_{oral}) for sum PAH4 EFSA [ng/kg/d]					3.87E-04	2.06E-06			**7.97E-10**
Inhalation general population	Regional PEC in air (total) [ng/m³]	1.08E-09						lung	3.00E-05	**3.24E-14**
								bladder	2.10E-05	**2.27E-14**
		1.23E-03						total (lung & bladder)		**5.51E-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 6% to the overall oral exposure, which is locally (Table 9-32) and regionally (Table 9-33) dominated by uptake of PAHs via fish.

The high fraction of PAHs in fish comes from the high BCF values of the PAHs, which are expected to accumulate in fish.

Table 9-32: 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	5.45E-02	7.37E-01	1.38E-01	1.01E-03	4.62E-02	2.26E-02	9.96E-04	1.00
Chrysene	3.14E-03	9.95E-01	8.55E-04	3.00E-05	4.35E-04	2.13E-04	6.25E-06	1.00
Benzo[a]pyrene	3.04E-02	9.60E-01	1.06E-03	5.76E-04	5.23E-03	2.55E-03	2.57E-05	1.00
Benzo[b]fluoranthene	5.32E-04	9.99E-01	8.19E-05	2.79E-05	1.21E-04	5.91E-05	7.00E-07	1.00

Table 9-33: 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	5.98E-02	8.09E-01	1.70E-02	9.40E-02	1.34E-02	6.53E-03	1.23E-04	1.00
Chrysene	3.13E-03	9.92E-01	5.44E-04	4.01E-03	4.51E-04	2.20E-04	3.93E-06	1.00
Benzo[a]pyrene	2.74E-02	8.65E-01	2.79E-03	8.94E-02	1.00E-02	4.89E-03	6.59E-05	1.00
Benzo[b]fluoranthene	5.27E-04	9.90E-01	1.22E-03	6.72E-03	1.00E-03	4.90E-04	1.04E-05	1.00

Although representative food consumption data of the German population were used instead of the very conservative EUSES default values, the oral intake calculations remain conservative (the conservatism 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 come 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). Since all water emissions from formulation activities at RÜTGERS Germany are discharged into the Emscher River and from that after short distance into the Rhine it can reasonably be assumed that a low portion of the emitted substances come into contact with areas where food is produced.

- The same holds true for the consumption of fish. In EUSES it is considered that 100% fish caught in the Emscher River are consumed by the local population (according to the necessary adjustments due to water emissions into the marine environment; as described in the input parameters for EUSES modelling in section 9.1.2.3). However, in reality, commercial fishing in the Emscher River is non-existent and recreational fishing also close to nil nowadays. In the future, when the Emscher River will be recultivated, it will probably take years up to decades until fish populations are established, which may then be available for fishing.

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 Emscher River)

The following tables provide the final risk calculation for the local (Table 9-34) and regional (Table 9-35) scenario.

Table 9-34: Calculation of excess life cancer risks (ELCRs): local assessment

Exposure route	Source / justification	ELCR
Oral **general population**	value calculated in Table 9-30 above, divided by factor 5:	**5.08E-08**
Inhalation **general population**	as calculated in Table 9-30 above: total (lung & bladder)	**6.17E-12**
Workers onsite (not involved in formulation activities)	as calculated in Table 9-30 above: total (lung & bladder)	**1.16E-12**

Table 9-35: Calculation of excess life cancer risks (ELCRs): regional assessment

Exposure route	Source / justification	ELCR
Oral **general population**	as calculated in Table 9-31 above	**7.97E-10**
Inhalation **general population**	as calculated in Table 9-31above: total (lung & bladder)	**5.51E-14**

Summary – Exposure and risks for man via the environment

The ELCRs indicate that the cancer risks for humans exposed via the environment to the formulation activities with CTPht are low due to the low exposure levels coming from the plant of RÜTGERS Germany. On the regional scale, ELCRs excess risk levels obtained are close to 1E-10. On the local scale, excess risk is dominated by consumption of fish from the Emscher River, which is actually close to zero for the large majority of the population. Despite the still relatively conservative modelling, calculated risks from local and regional exposure of humans via the environment are well below the 10^{-6} level for water and air emissions from formulation activities at RÜTGERS Germany.

9.1.3 Worker contributing scenario 1 – PROC 3 – PÖ-Mix Operators

9.1.3.1 Conditions of use

Table 9-36: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture: >50 - < 80 % CTPht • 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 • Air recovery system for truck loading stations
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 like sampling • Other PPE: standard safety equipment (working clothes, safety shoes, helmet with face shield or goggles)
Other conditions affecting workers exposure
• Place of use: Indoor/Outdoor • Operating temperature: ≤ [redacted]°C (in tasks related to potential exposure)

9.1.3.2 Exposure and risks for workers

<u>PÖ-Mix Operators:</u>

Operators carry out the following activities during their shifts:

- Control activities and documentation in the central control room
- Inspections of the technical equipment outside
- Sampling (outside) and
- analysis of small samples for softening point in dedicated lab room adjacent to control room
- Transport of large sample to central laboratory
- (Occasional) assistance for maintenance workers during repair work
- Communication with supervisors.

Sampling conditions at the tank farm PÖ-Mix (see also Figure 15-1 to Figure 15-12 in Annex IV – Photo documentation – Sampling):

- 1 large sample for central lab (200 mL) per shift
- Up to three small samples for determination of softening point (< 5 mL)
- Sampling takes place at dedicated sampling points (semi-enclosure) of the tank farm according to the work instruction described below, which has to be followed:

  - Prior to drawing a sample, the sampling container has to be checked for integrity. Damaged containers are disposed of.
  - The door of the sampling box at the sampling point is opened and the receiving plate pulled out only to the extent that the sampling vessel can be placed.
  - The sampling vessel is positioned with the help of the receiving plate under the outlet of the sampling device, so that the product can only run into the sampling vessel. The door of the sampling box is closed.
  - The sample vessel is filled by actuating the sampling valve. The filling process is constantly monitored by the sampler. When the desired amount of sample has been obtained, the sampling armature is closed again.
  - In the event of faults, sampling will be stopped immediately. If external conditions require sampling to stop, the sampling valve will be closed immediately.
  - A 5-minute waiting period must be allowed before removing the sampling vessel so that the product can cool down and solidify.
  - To remove the sampling vessel, the receiving plate is only removed so far that the vessel can be removed without difficulty.
  - If samples have been spilled during sampling, the sampling point must be cleaned after the product has cooled down! (Cleaning of spillage is performed by a specialised external company; workers are using adequate personal protective equipment.)
  - The cooled sample vessels are clearly assigned to a tank and a batch by means of sample stickers. The stickers also contain the product name and the labelling according to hazardous substances law.
- During sampling in addition to the basic protection equipment (see 9.1.1.4), operators wear gloves and respiration protection (protective equipment according to the operating instructions according to §14 GefStoffV for the sampling of liquid carbons).

Conditions of analysis of softening point of small sample (see also Figure 17-1 and Figure 17-2 in Annex VI – Photo documentation – On-site analytics):

- Maximum three times per shift
- Analysis of small probe (few mL) below ventilation hood
- During the analysis the workers wear the basic PPE (i.e. work suit, safety shoes S3, goggles with side protection but no helmet with face shield, and in addition protective gloves according to glove plan, i.e. disposable nitrile glove under protective leather glove)
- Any waste is disposed in the so-called pitch container, which goes to waste intermediate storage (AZL) and is subsequently disposed of (incineration).

<u>Foremen (“Anlagenvorarbeiter”) and other workers:</u>

Foremen are supervising work in all units in the northern part of the production site. They are mainly working inside the central control room with occasional inspections of various places in the northern part of the site.

Their time outdoors close to the PÖ-Mix tank area or the dedicated filling stations is estimated to be around 5% of their shift (i.e. 30 min per shift). However they are not assigned any specific activity with potential exposure.

Other workers (n=4) related to PÖ-Mix unit are supervisors (“Anlagenmeister”, n=2), one technician, and one head of operation, all working in the northern part in day shifts (8 h/d, 5 d/w). Mostly their work is inside the control room or relevant other buildings on the facility. Occasionally they perform inspections of the activities performed and technical equipment outside. Their time outdoors close to the PÖ-Mix tanks area or the dedicated filling stations is estimated to be around 5% of their shift (i.e. 30 min per shift). Comparable to foremen they are not assigned any specific activity with potential exposure.

Description of data used for assessment of workers’ exposure

Inhalation exposure

Air measurements:

Some personal samples (air measurements) are available at RÜTGERS Germany, from samples analysed on several occasions between 2006 and 2010.

Table 9-37: Exposure concentrations of benzo[a]pyrene from personal air sampling (year 2006 – 2010; method of determination: PAS-Langzeit/NIOSH 5515)

Date	Measured concentration [µg/m³]	Measuring period [h]	Measuring period [min]	Exposure period [h/shift]	Exposure shift mean [µg/m³ per 8h]
06.07.2006	0.04	6.33	380	6.5	0.0325
10.07.2006	<0.01	4.95	297	6.5	< 0.01
10.07.2006	0.04	6.10	366	6.5	0.0325
09.08.2007	0.06	6.25	375	6.5	0.049
17.02.2010	<0.03	2.67	160	6.5	<0.03

In addition to this air sampling a biomonitoring campaign was performed recently. Samples were taken from different groups of workers in September 2018. All raw data are presented in separate file in IUCLID section 13. Further details are provided in Annex XII – Biomonitoring Campaign.

Samples were taken at the end of shift. Importantly, all samples were taken contamination free. This means that specimen collection was performed after taking off the work clothes and washing hands or showering at the end of the activities involved. Collection was carried out directly in the urine cup. Most participating workers provided more than 1 sample.

There are a total of 12 PÖ-Mix operators. Six of them volunteered for the biomonitoring campaign and delivered 22 samples in total. Four of the operators were smokers (see Table 9-38).

Table 9-38: Results from biomonitoring campaign of 6 PÖ-Mix operators in September 2018; values are given as 1-hydroxypyrene in urine (µg 1-OHP/g creatinine), measured after end of shift

	# of operators	# of measurements	arithm. mean	max	90th percentile
total	6	22	1.7	5.5	2.5
smoker	4	13	2.0	5.5	4.0
non-smoker	2	9	1.3	2.5	2.3

Two high values (5.5 and 4.0 µg 1-OHP/g creatinine) were observed with one individual operator (smoker), who had much lower values (1.2 and 2.5 µg 1-OHP/g creatinine) at two further time points.

Besides operators also foremen ("Anlagenvorarbeiter") are active in the PÖ-Mix facility. A total of 6 foremen are working at RÜTGERS Germany. The following table provides biomonitoring data available for this group. Two foremen participated in the campaign and delivered 9 samples in total.

Table 9-39: Results from biomonitoring campaign of 2 foremen in September 2018; values are given as 1-hydroxypyrene in urine (µg 1-OHP/g creatinine), measured after end of shift

	# of operators	# of measurements	arithm. mean	max	90th percentile
total	2	9	0.6	1.1	0.9
smoker	0	0	0	0	0
non-smoker	2	9	0.6	1.1	0.9

As expected from their job description (work mainly in the control room), foremen show significantly lower exposure levels compared to operators.

Although the database depicts some variability, the overall database on all groups of workers shows that smokers had consistently higher levels (by approx. factor around 2). Yet, in order to have sufficient measurements available all workers of each job group are included for the exposure assessment. 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.

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 (BaP conc.) the equation as given in ECHA (2018) is used:

$$\textbf{BaP conc.}\,[\textbf{ng/m}^3] = \frac{(\textbf{1– OHP urinary concentration }[\mu\textbf{mol/mol creatinine}] - \textbf{1.13})}{\textbf{11.1}}$$

In the following table 90th percentile values for the two different groups of workers as shown in Table 9-40 are converted into BaP air concentrations.

Table 9-40: 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)
PÖ-Mix operators	2.5	1.30	14.9
Foremen	0.9	0.48	-

The workers at PÖ-Mix are currently only handling formulations during a very limited time of their yearly working time, as they otherwise handle pure CTPht. In the future this might change and up to a total of [redacted] (20-100)% of the production volume might be formulated. [redacted]

Table 9-41: Excess lifetime cancer risks (ELCRs) for operators (n = 12 workers)

Target organ:	Long-term exposure [ng BaP/m^3] *	[redacted]	corrected concentration [ng BaP/m^3]	Risk estimate for cancer per 1 ng BaP/m^3 (40 years of occupational exposure)	ELCR
	14.9	[redacted]	10.9		
Lung				5.60E-06	6.10E-05
Bladder				4.00E-06	4.36E-05
Combined					1.05E-04

Unrounded values used for calculation.

No excess risks are calculated for foremen. 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 0.48 µmol/mol creatinine), it can be reasonably assumed that their exposure is not far from background exposure levels.

Remarks on exposure data and discussion:

The data in Table 9-38 show that on average workers of the PÖ-Mix unit have 1-OHP values below 1.7 µg/g creatinine (or 0.88 µmol/mol creatinine). 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 value shows that occasionally higher exposures might occur. By using the 90th percentile value 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.

From years 2006 to 2010 some (personal) air monitoring data are available. Concentrations ranged from below 10 ng/m³ BaP to 49 ng/m³ BaP. This fits well to the estimated BaP exposure levels based on biomonitoring data, especially if the improvements achieved during the last years are taken into account. The comparison also allows to conclude that no relevant dermal exposure occurs at these workplaces.

90th percentile biomonitoring values are used for risk characterisation. With these conservative assumptions the calculated combined ELCR for PÖ-Mix operators is at 1.05 x 10^{-4}, taking into account the actual time spent on formulation activities.

Foremen seem to have slightly elevated PAH exposure levels (AM 0.6, 90th perc. 0.9 µg 1-OHP/g creatinine), which are not far from background levels for the general population in Germany: 90th percentile measured in non-smokers (n = 278) is 0.2 µg 1-OHP/g creatinine and 0.5 µg 1-OHP/g creatinine in smokers (n = 184) (Becker et al., 2003). Internal controls at RÜTGERS Germany from three individuals (all non-smokers) showed very low levels of <0.1 to 0.04 µg/g creatinine. Anyway, foremen spend only a very limited fraction of their total working time on supervising activities related to production of formulations.

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 (up to [redacted]°C), which would immediately cause severe burns
- the company's medical history documents that such incidents are extremely rare (10 cases for tasks related to CTPht or AO in the whole plant in the last 5 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.

The comparison with the available personal air monitoring data confirm that the contribution from dermal exposure is negligible.

Conclusion on risk characterisation:

Calculated extra cancer risks are

operators (n = 12): 1.05×10^{-4}

foremen (n = 6) and other workers (n = 4): negligible

9.1.4 Worker contributing scenario 2 – PROC 3 – Ölbetrieb Operators

9.1.4.1 Conditions of use

Table 9-42: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture:> 50 - < 80% CTPht • 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 • Air recovery system for truck loading stations
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 like sampling • Other PPE: standard safety equipment (working clothes, safety shoes, helmet with face shield or goggles)
Other conditions affecting workers exposure
• Place of use: Outdoor • Operating temperature: ≤ [redacted]°C (in tasks related to potential exposure)

9.1.4.2 Exposure and risks for workers

<u>Ölbetrieb Operator:</u>

Operators carry out the following activities during their shifts:

- Control activities and documentation in the central control room
- Outside realization of the product routes for an operational production process via manual manipulation of valves (e.g. product flaps, slides, ball valves, etc.)
- Inspections of the technical equipment outside
- Sampling (outside)
- Transport of large sample to central laboratory
- (Occasional) assistance for maintenance workers during repair work
- Communication with supervisors.

Sampling conditions at relevant Ölbetrieb tanks (comparable to PÖ-Mix, see Figure 15-1 to Figure 15-12 in Annex IV – Photo documentation – Sampling):

- 6 to 10 samples from different tanks and products (sample size from 250 to 1000 mL) for central laboratory analysis per shift
- Sampling takes place at dedicated sampling points (semi-enclosure) according to the applicable work instruction, which has to be followed:
    - The door of the sampling box at the sampling point is opened.

- A vessel is screwed into the sampling holder or pressed by means of a lifting table and the sampling box is closed.
- The sampling valve is opened and the liquid sample taken (duration about 1 min).
- The door of the sampling box is opened, the vessel is taken out and then closed. Subsequently the samples are taken to the central laboratory for evaluation.
- During sampling respective PPE is worn: i.e. AlphaTec gloves, full mask with AEBK filters, helmet, working clothes and safety shoes S3

Note that currently no CTPht is handled at Ölbetrieb. But from 2019 onwards it is planned to manufacture carbon black feedstock containing CTPht and oil fractions from the coal tar distillation. Therefore, Ölbetrieb operators are included here.

Foremen (“Anlagenvorarbeiter”) and other workers:

As these are the same workers already described in WCS1 and their exposure was already assessed in section 9.1.3 these workers will not be considered further in WCS2.

Description of data used for assessment of workers’ exposure

Inhalation exposure

Air measurements:

Some personal samples (air measurements) from operators from “Ölbetrieb” north are available at RÜTGERS Germany, from samples analysed between 2007 and 2015.

Table 9-43: Exposure concentrations of benzo[a]pyrene from personal air sampling (2007 – 2015; method of determination: PAS-Langzeit/NIOSH 5506)

Datum	Measured concentration [µg/m³]	Measuring period [h]	Measuring period [min]	Exposure period [h/shift]	Exposure shift mean [µg/m³ per 8h]
07.11.2007	< 0.04	5.58	335	6.0	<0.04
17.02.2010	< 0.02	6.83	410	6.0	<0.02
05.09.2011	0.02	6.93	416	6.0	0.015
29.07.2013	< 0.01	6.92	415	6.0	<0.01
16.09.2015	< 0.02	6.27	376	6.0	<0.02

In addition to this air sampling a biomonitoring campaign was performed recently. Samples were taken from different groups of workers in September 2018. All raw data are presented in separate file in IUCLID section 13. Further details are provided in Annex XII – Biomonitoring Campaign.

Samples were taken at the end of shift. Importantly, all samples were taken contamination free. This means that specimen collection was performed after taking off the work clothes and washing hands or showering at the end of the activities involved. Collection was carried out directly in the urine cup. Most participating workers provided more than 1 sample.

There are a total of 6 Ölbetrieb operators. Three of them volunteered for the biomonitoring campaign and delivered 10 samples in total. One of the operators was a smoker (see Table 9-44).

Table 9-44: Results from biomonitoring campaign of 3 Ölbetrieb operators in September 2018; values are given as 1-hydroxypyrene in urine (µg 1-OHP/g creatinine), measured after end of shift

	# of workers	# of measurements	arith. mean	max	90th percentile
total	3	10	1.03	2.40	1.86
smoker	1	3	1.93	2.40	2.28
non-smoker	2	7	0.65	0.82	0.78

Although the database depicts some variability, the overall database on all groups of workers shows that smokers had consistently higher levels (by approx. factor 2). Yet, in order to have sufficient measurements available all workers of each job group are included for the exposure assessment. 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.

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 (BaP conc.) the equation as given in ECHA (2018) is used:

$$\mathbf{BaP\ conc.}\,[\mathbf{ng/m^3}] = \frac{(\mathbf{1\text{–}\ OHP\ urinary\ concentration}\ \ [\boldsymbol{\mu}\mathbf{mol/mol\ creatinine}] - \mathbf{1.13})}{\mathbf{11.1}}$$

In the following table 90th percentile value for the Ölbetrieb operators as shown in Table 9-45 is converted into BaP air concentration.

Table 9-45: 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)
Ölbetrieb operators	1.86	0.96	-

As described above, currently these workers are not exposed to any (formulation) activities including CTPht. Therefore, these measurements cannot be used for the assessment.

As expected their exposure levels are lower than those of PÖ-Mix operators. As their 1-OHP levels are below 1.13 µmol/mol creatinine (90th percentile 0.96 µmol/mol creatinine), no corresponding BaP workplace air concentration and no excess risks can be calculated. This is in agreement with existing personal air workplace measurements, which are mostly below the limit of quantification (Table 9-45).

In order to account for the potential future production of formulations at the Ölbetrieb installations, BaP exposure levels are taken from currently exposed PÖ-Mix operators (cf. Table 9-40). As job description is similar, similar exposure levels are likely in case formulation activities with CTPht would take place in Ölbetrieb as well. Note: currently PÖ-Mix operators are also handling only a minor amount of formulations, during the remaining time they handle pure CTPht.

However, as the tonnage of CTPht envisaged for formulations from Ölbetrieb is lower than the tonnage anticipated to be used in PÖ-Mix the time Ölbetrieb operators would handle formulations is shorter than for PÖ-Mix workers. This has to be taken into account, resulting in lower long-term average exposure levels for Ölbetrieb operators. [redacted]

Table 9-46: Excess lifetime cancer risks (ELCRs) for Ölbetrieb operators (n = 6)

Target organ:	Long-term exposure [ng BaP/m³]	[redacted]	corrected concentration [ng BaP/m³]	Risk estimate for cancer per 1 ng BaP/m³ (40 years of occupational exposure)	ELCR
	14.9	[redacted]	0.90		
Lung				5.60E-06	5.02E-06
Bladder				4.00E-06	3.58E-06
Combined					8.60E-06

Unrounded values used for calculation.

Besides Operators also foremen (“Anlagenvorarbeiter”) are active in the Ölbetrieb. As these are the same workers as already described in Worker CS 1 (in section 9.1.3) from the PÖ-Mix facility their possible ELCR is already discussed above. The same is true for additional workers shared between these two facilities and that are not described in the worker contributing scenarios in the following sections.

Remarks on exposure data and discussion:

As explained above using the 90th percentile value for the risk characterisation is a conservative approach as it assumes that

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

90th percentile biomonitoring values as measured for PÖ-Mix operators, but with adjustment of the increased working time of Ölbetrieb operators handling larger CTPht volumes in the future, are used for risk characterisation. With these conservative assumptions the calculated combined ELCR for Ölbetrieb operators is at 8.60×10^{-6}, taking into account the actual time spent on formulation activities.

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 (up to [redacted]°C), which would immediately cause severe burns
- the company's medical history documents that such incidents are extremely rare (10 cases for tasks related to CTPht or AO in the whole plant in the last 5 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.

The comparison with the available personal air monitoring data confirms that the contribution from dermal exposure is negligible (see WCS1). Also the data from Ölbetrieb operators show that dermal exposure at these workplaces is negligible. 1-OHP levels in urine were slightly elevated, but below 1 µmol/mol creatinine. Four out of 5 existing workplace air measurements from years 2007 to 2015 were below the LOQ (below 10 - 40 ng/m^3 BaP), with one value measured at 15 ng/m^3 BaP.

Conclusion on risk characterisation:

Calculated extra cancer risks are

operators (n = 6): 8.60×10^{-6}

foremen (n = 6) and other workers (n = 4): assessment in WCS1 in section 9.1.3 as these are the same workers

9.1.5 Worker contributing scenario 3 – PROC 8b – PÖ-Mix: Tank truck loading and Ölbetrieb - central oil loading: Tank truck/rail tank car loading

9.1.5.1 Conditions of use

Table 9-47: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture: >50 - < 80% CTPht • 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 • Air recovery system for truck/rail tank car loading stations
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: No (but after completed loading workers wear respirator (full mask) with ABEK filter or respirator with hose) • Other PPE: standard safety equipment (working clothes, safety shoes, helmet with face shield or goggles)
Other conditions affecting workers exposure
• Place of use: Outdoor • Operating temperature: ≤ [redacted]°C (in tasks related to potential exposure)

9.1.5.2 Exposure and risks for workers

Tank trucks/rail tank cars are loaded at dedicated loading stations. Six loading operators are in charge of operations at both loading stations.

Technical description:

<u>PÖ-Mix:</u>

- Dedicated loading station for trucks with extraction of exhaust air into the slop system BS10.1
- Before automated filling process of PÖ-Mix products at the dedicated loading station for trucks can be started, all necessary positions of the security chain must be fulfilled, i.e. position of the loading arm, pressure of the arm, ground cable at the truck connected, emergency unlocked, the truck needs to have a filling level below maximum level.

Currently approximately [redacted](1 000-20 000) tank trucks are loaded per year (total transport capacity approx. [redacted] (25 000-500 000)t). Thereof only less than [redacted] (1-50)% are containing CTPht/oil mixtures, which are in the scope of this application for authorisation. Approximately [redacted] (50-100)% of tank trucks are loaded with CTPht neat[15] and the remaining [redacted] (1-50)% are liquid products not contributing to PAH exposure.

In the future the amount of relevant mixtures loaded via the PÖ-Mix loading facilities will increase. The total transport capacity will not be changed. [redacted]

<u>Ölbetrieb → central oil loading facility:</u>

- Dedicated loading station for trucks/rail tank cars with extraction of exhaust air via the loading arms
- Before automated filling process of Ölbetrieb products a similar security chain must be activated as described above for PÖ-Mix above.

Approximately [redacted] (1 000-10 000) tank trucks / rail tank cars are loaded per year. In 2018, thereof only less than [redacted] (1-50)% were containing AO + CTPht mixtures, which are in the scope of this application for authorisation. However this could increase when more CTPht is used for CBO mixtures. [redacted] 50% of this higher product output would be loaded in the central oil loading facility [redacted]

<u>Summary:</u>

- **Current situation:**
    - PÖ-Mix: [redacted]
    - Central oil loading facility: [redacted]
    - <u>Combined:</u> Loading operators handle a total of [redacted] (2 000-30 000) tank trucks / rail cars. Thereof less than [redacted] (1-50)% contain CTPht/oil mixtures (relevant for this authorisation). Yet also CTPht neat is loaded (i.e. [redacted] (30-85)% of all tank trucks). Thus a total of [redacted] **(30-100)% of all loading operations contribute to the PAH exposure**.
- **In the future:**
    - PÖ-Mix: [redacted]
    - Central oil loading facility: [redacted]
    - <u>Combined</u>: Loading operators will handle a total of [redacted] (2 000-30 000)tank trucks / rail cars Thereof approx. [redacted] (30-85)% contain CTPht/oil mixtures (relevant for this AfA). In addition a minor fraction of CTPht neat is loaded (i.e. [redacted] (1-50)% of all tank trucks). Thus a total of [redacted] **(30-100)% of all loading operations contribute to the PAH exposure**.

Regardless of the loading station in each loading operation there are two workers involved:

- <u>Truck driver</u> (see also Figure 16-1 to Figure 16-3 in Annex V – Photo documentation – Loading PÖ-Mix):

The truck driver is in charge of opening the manhole on top of the truck. All other tasks are performed by the loading operator. After opening the manhole the truck driver is obliged to

[15] CTPht neat is also transported via barge ships see WCS4 in section 9.1.6

retreat to an observation station in about 20 m distance (general PPE (according to transport of dangerous goods regulations, ADR), no exposure).

- Loading operator (see also Figure 16-4 to Figure 16-8 in Annex V – Photo documentation – Loading PÖ-Mix):

The following activities are performed by the loading operator and measures taken to reduce exposure:

- visual inspection of the condition of the tank car
- entering of the loading station
- visual inspection interior of the container through the opened manhole (duration approx. 2 min.).
- Placement of loading arm with nozzle by hydraulic remote control (duration approx. 3 min).
- loading arm equipped with exhaust ventilation to prevent emissions to air
- leaving of loading station → automatic filling (only possible if security chain is activated) → loading duration approx. 1 hour
- afterwards the operator removes the loading arm by remote control out of the manhole (total duration approx. 5 min)
- nozzle situated above the manhole for allowing dripping (200 seconds waiting period required)
- emptying of filling line on-site happens automatically (PÖ-Mix - on the container BS24)
- moving loading arm to its resting position
- exhaust ventilation (via the slop system ([redacted]) at PÖ-Mix) for exhaust gases during loading → thus no emission to air

During these activities, the staff / truck driver (according to transport of dangerous goods regulations, ADR) will wear basic PPE and in addition, gloves according to the glove plan (i.e. Ansell AlphaTec 58-535, for respective breakthrough times cf. Annex VIII – Breakthrough times according to RÜTGERS Germany glove plan).

Description of data used for assessment of workers' exposure

Inhalation exposure

A biomonitoring campaign was performed recently. Samples were taken from different groups of workers in September 2018. All raw data are presented in separate file in IUCLID section 13. Further details are provided in Annex XII – Biomonitoring Campaign.

Samples were taken at the end of shift. Importantly, all samples were taken contamination free. This means that specimen collection was performed after taking off the work clothes and washing hands or showering at the end of the activities involved. Collection was carried out directly in the urine cup. Most participating workers provided more than 1 sample.

There are a total of 6 loading operators responsible for the loading operations at the PÖ-Mix loading station as well as the central oil loading facility (loading operations from Ölbetrieb).

Two of them volunteered for the biomonitoring campaign and delivered 7 samples in total. One of the operators was a smoker the other one a non-smoker (see Table 9-48).

Table 9-48: Results from biomonitoring campaign of 2 loading operators in September 2018; values are given as 1-hydroxypyrene in urine (µg 1-OHP/g creatinine), measured after end of shift

	# of workers	# of measurements	mean	max	90th percentile
total	2	7	0.88	1.50	1.44
smoker	1	4	1.21	1.50	1.47
non-smoker	1	3	0.45	0.68	0.63

Although the database depicts some variability, the overall database on all groups of workers shows that smokers had consistently higher levels (by approx. factor around 2). Yet, in order to have sufficient measurements available all workers of each job group are included for the exposure assessment. 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.

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 (BaP conc.) the equation as given in ECHA (2018) is used:

$$\mathbf{BaP\ conc.}\,[\mathbf{ng/m^3}] = \frac{(\mathbf{1\text{–}\ OHP\ urinary\ concentration\ \ [\mu mol/mol\ creatinine]\ –\ 1.13})}{\mathbf{11.1}}$$

In the following table 90th percentile value for the loading operators as shown in Table 9-49 is converted into BaP air concentration.

Table 9-49: 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)
loading operators	1.44	0.75	-

No excess risks are calculated for loading operators. Their exposure levels are low and thus their 1-OHP levels are below 1.13 µmol/mol creatinine (90th percentile 0.75 µmol/mol creatinine), it can be reasonably assumed that their exposure is not far from background exposure levels.

Remarks on exposure data and discussion:

The data in Table 9-48 show that on average loading operators, responsible for all loading activities from PÖ-Mix and Ölbetrieb, have 1-OHP values below 0.88 µg/g creatinine (or 0.46 µmol/mol creatinine) and even the 90th percentile is below 1.44 µg/g creatinine (or 0.75 µmol/mol creatinine). According to RACs exposure-risk relationship these values relate 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).

As explained above using the 90th percentile value for the risk characterisation is a conservative approach as it assumes that

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

In addition, from all loading operations performed by the loading operators currently only around [redacted] (1-50)% are related to formulations relevant for this AfA.

In the future the amount of relevant CTPht/oil mixtures will increase. Yet the exposure is not anticipated to increase drastically as biomonitoring data available account for exposure to CTPht/oil mixtures as well as CTPht neat, which is also handled by the logistics operators. As outlined above currently approximately [redacted] (30-100)% of all loading operations contribute to the PAH exposure measured due to CTPht handling. In the future this will only increase by a small percentage (i.e. total of [redacted] (30-100)% of all loading operations) when loading operators will handle more mixtures instead of neat CTPht. This slight increase is anticipated to only marginally increase the measured very low exposure levels of PAHs. The currently measured 90th percentile of 1-OHP levels (0.75 µmol/mol creatinine) are well below the level at which RAC assumes relevant workplace exposures to start. Thus it is assumed that the minor increase in PAH exposure will lead to minor increase of 1-OHP values, still well below 1.13 µmol/mol creatinine and thus cancer risk will still be negligible.

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 (up to [redacted]°C), which would immediately cause severe burns
- the company's medical history documents that such incidents are extremely rare (10 cases for tasks related to CTPht or AO in the whole plant in the last 5 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

loading operators (n = 6): negligible

9.1.6 Worker contributing scenario 4 – PROC 8b – Barge (ship) loading

9.1.6.1 Conditions of use

Table 9-50: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture: >50 - < 80% CTPht • 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 • Air recovery system for barge (ship) loading arm
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: No • Other PPE: standard safety equipment (working clothes, safety shoes, helmet with face shield or goggles)
Other conditions affecting workers exposure
• Place of use: Outdoor • Operating temperature: ≤ [redacted]°C (in tasks related to potential exposure)

9.1.6.2 Exposure and risks for workers

Barges are loaded at the dedicated loading station (liquid port) via loading arms.

Technical description:

- Dedicated loading arm (RXL-VB-01) with extraction of exhaust air (via scrubber in oil storage 3 to exhaust gas combustion facility, AVS).
- The following process parameters apply to loading of barges via the dedicated loading arm:
    - min. loading temperature: 40 °C,
    - max loading temperature: 150 °C,
    - max. permissible pressure for piping system: 8 bar, and
    - max. flow rate: 250 - 300 t/h
- Before automated filling process of Ölbetrieb products at the dedicated loading station for barges are started, the security chain must be activated (i.e. manual start-up and disconnect protection (called MATS) in the local control room (see Figure 9-7), locking of loading arm, level measurements installed, etc.).
- Since cargo holds of the barges have no continuous level measurements, the loading can be performed according to two variants:
    1. The masses for loading the barge can be specified in the PLS, and are detected with a Coriolis mass flowmeters (CMD). Via potential-free alarm contacts the

loading of the barge can be switched off timely on reaching the specified set point.
2. The volumes for loading the barge can be communicated between the operator on-site and the process operator at the central control room, both of which are in constant contact (telephone, radio). The loading of the barge to the desired level is monitored via camera by the central control room (automated PLS system).

In addition, barges used have overfill prevention systems available in the loading chambers. These automatically interrupt the charging process via the connected safety chain.

- Loading arm is generally maneuvered via hydraulic remote control (RÜTGERS worker at land uses use panel 1, ship's crew uses use panel 2 installed at the head of the loading arm).

Loading operations at the liquid port:

- Maximum amount charged: 1000-1200 tonnes per barge
- Approx. [redacted] (1-30) barges per week are loaded (i.e. around [redacted] (52-1 500) barges per year)
- Currently only a minor fraction of the mixtures shipped contain CTPht, but there might be shifts in products and this higher amount of relevant products is estimated and considered relevant for this assessment
    - From PÖ-Mix: the potential maximum tonnage of [redacted] (25 000-400 000) t CTPht for hybrid pitch results in [redacted] (30 000-530 000) t of product [redacted]. 50% of this product output would be shipped via barges. [redacted] For this assessment [redacted] (30-450) barges (i.e. calculated mean of minimum and maximum number of barges) will be assumed. [redacted].
    - From Ölbetrieb: the potential maximum tonnage of [redacted] (5 000-100 000) t CTPht for formulation results in approx. [redacted] (10 000-250 000) t of product [redacted]. 50% of this product output would be shipped via barges[redacted] For the [redacted] (5 000-125 000) t a maximum of [redacted] (5-125) barges are required for transportation[redacted].
    - **Total:** [redacted] (20-80) % of all barges contain mixtures relevant for this assessment.
- Barge loading process takes generally approx. 4 to 5 hours (approx. 250 to 300 t/h).
- Tasks associated with potential exposure take only a few minutes.

Workers:

- **one worker** (member of the RÜTGERS Germany fire brigade) which provides the loading arm (attached by ship's crew)
- **one operator/foreman** from Ölbetrieb present in order to document the process with signature and to open the pusher coming from the relevant tanks
- They start and stop the loading process from >4 m distance.

A schematic of the situation at the liquid port is provided in Figure 9-7 below.

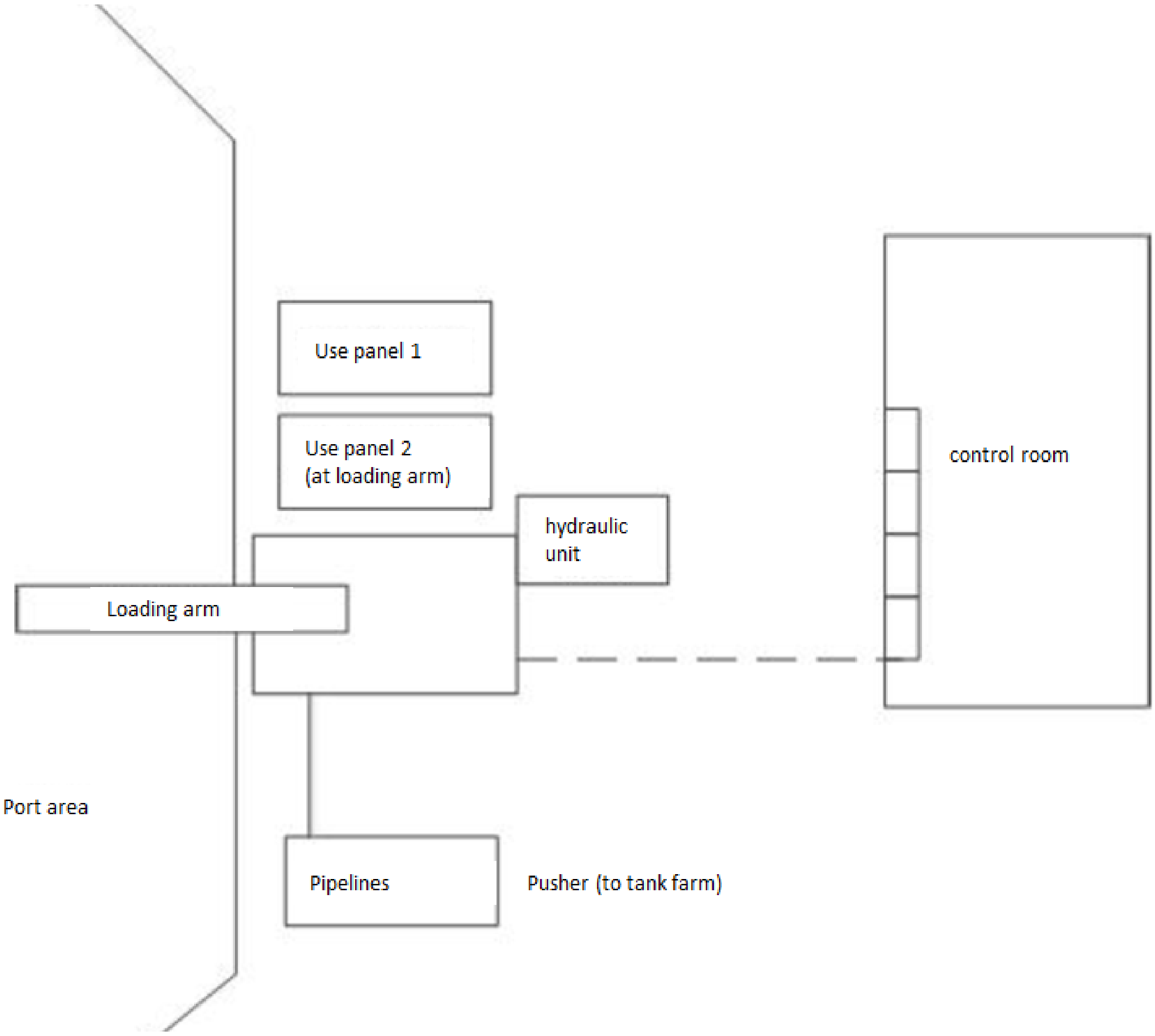

Figure 9-7: Scheme of the liquid port

The process has suction via the exhaust line (exhaust gas combustion facility, AVS).

Additional safety precautions taken are, e.g. camera surveillance of the process, general surveillance via process control system (PLS), Emergency Stop in central control room, ADN Checklist, and a detailed work instruction (written) is provided. All workers wear general PPE (helmet, gloves, safety shoes, work clothes, but no mask).

After loading, the lines are blown with nitrogen to remove residue. If additional residues remain in the pipe, they will be transferred to the drip pan of the ship in the next charging process. Disposal will be performed by ship's crew.

Description of data used for assessment of workers' exposure

Inhalation exposure

Operator/foreman from Ölbetrieb

These workers have only documentation tasks during ship loadings. No relevant exposure is expected for them. Other exposures and the resulting ELCR for Ölbetrieb operators and foremen from the Ölbetrieb were discussed already in section 9.1.4. No further assessment will be performed.

RÜTGERS Germany fire brigade worker

In total there are 40 fire brigade workers. 19 of them are only working part-time. The remaining 21 fire brigade workers are employed full-time by RÜTGERS Germany and carry out e.g. the loading activities in the liquid port.

As for these 21 fire brigade workers there are no personal air measurements or biomonitoring data available exposure concentration of benzo[a]pyrene was modelled with the Advanced REACH Tool (ART). The input parameters used for ART modelling are shown in Table 9-51. The task modelled with ART is related to the phase when loading is started and the fire brigade worker is leaving the liquid port (task duration 3 minutes). The full protocol is documented in Annex XIII – ART Protocol.

Table 9-51: Input parameters used for exposure modelling of fire brigade workers during barge loading

Parameter	Selected
Activity	Transfer of substance from/to large containers at dedicated facility (PROC 8b, barge loading, far field)
Temperature	[redacted] °C
Vapour pressure	0.98 Pa (see section 9.0.3.3)
Weight of fraction of the substance in the liquid mixture	0.00873
Viscosity	Liquids with medium viscosity (like oil)
Primary emission source located in the breathing zone of the worker?	No
Activity class	Transfer of liquid products
Transfer of liquid product with flow of:	>1 000 L/min [b]
Level of containment of the process?	Open process [b]
Transfer of liquid performed by splash or submerged loading?	Splash loading, where the liquid dispenser remains at the top of the reservoir and the liquid splashes freely
Control measures in close proximity of the far-field emission source?	Vapour recovery systems

Secondary control measures in close proximity of the far-field emission source	No secondary localised controls
Emission source segregated from the work environment by isolation of the source in a segregated room or work area?	No segregation
Worker separated from the emission source(s) by means of a personal enclosure around the worker (e.g. cabin)?	No personal enclosure
Process fully enclosed and is the integrity of that enclosure regularly monitored?	No
Demonstrable and effective housekeeping practices in place (e.g. preventive maintenance of machinery, use of protective clothing)?	Yes
Where is the work performed?	Outdoors

As there are [redacted] (1-30) barges loaded per week only one loading activity is modelled per shift. Fire brigade workers are not assigned any other task related to CTPht/oil mixtures (relevant for this AfA). Starting the procedure is the only task associated with potential exposure; this should only take a few seconds. When the loading is started the fire brigade worker will leave the liquid port and only return when loading is already finished to manoeuvre the loading arm into the resting position. Thus total exposure duration of 3 minutes was assumed and the total shift length of 480 minutes considered when the exposure concentration was estimated.

As outlined before around [redacted] (20-80)% of all barges loaded might contain mixtures relevant for this AfA. This circumstance is considered when allocation the excess lifetime cancer risks (see Table 9-52). In addition another correction factor was introduced which considers that each fire brigade worker is working on 220 days per year only, but up to [redacted] (52-1 500) barges are loaded per year which require only one worker per loading.

Table 9-52: Excess lifetime cancer risks (ELCRs) for fire brigade worker (n = 21)

Target organ:	Exposure conc. predicted in ART - TWA [ng BaP/m^3]*	[redacted]	Frequency correction factor**	Long-term exposure (corrected concentration) [ng BaP/m^3]	Risk estimate for cancer per 1 ng BaP/m3 (40 years of occupational exposure)	ELCR
	0.19	[redacted]	0.06	0.007		
Lung					5.60E-06	3.96E-08
Bladder					4.00E-06	2.33E-08
Combined						6.79E-08

* Exposure air concentration modelled with Advanced REACH Tool
** Frequency correction factor: Loading operations for each individual operator [redacted]

Remarks on exposure data:

As no air measurements or biomonitoring data available exposure concentration of benzo[a]pyrene was modelled with the Advanced REACH Tool (ART). Exposure models are designed to provide a conservative result to account for the uncertainties inherent in modelling. Based on the BaP air concentration calculated, a low ECLR of 6.79×10^{-8} is assumed for the fire brigade workers involved in barge loading. Determining a low risk for fire brigade workers is not surprising with the low period of time in which an exposure seems possible. In addition the low exposure calculated seems reasonable as loading process in the liquid port are somewhat comparable to activities performed by logistics operators in charge of loading in PÖ-Mix and central oil loading facilities. Here the results of the biomonitoring data obtained, confirm the low exposure assumed for this task.

Dermal exposure

As outlined for all other exposure scenarios 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 (up to [redacted]°C), which would immediately cause severe burns
- the company's medical history documents that such incidents are extremely rare (10 cases for tasks related to CTPht or AO in the whole plant in the last 5 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

Fire brigade worker (n = 21): 6.79×10^{-8}

9.1.7 Worker contributing scenario 5 – PROC 15 – Laboratory technicians

9.1.7.1 Conditions of use

Table 9-53: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture:>50 - < 80% CTPht • Physical form of the used product: solid / 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 (standard efficiency)
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: No • Other PPE: standard safety equipment (laboratory coat, working pants, safety shoes, goggles)
Other conditions affecting workers exposure
• Place of use: Indoor • Operating temperature: room temperature to ≤ [redacted]°C (in tasks related to potential exposure; exception: QI analysis in closed shaking bath at [redacted]°C and carbon residue measurements at [redacted]°C)

9.1.7.2 Exposure and risks for workers

<u>Laboratory workers:</u>

The central laboratory facility is currently divided in three sections. There will be restructuring in the near future. In general, all of the sections are in contact with CTPht/oil and CTP/AO formulations during their work. During the remaining time they work on analysis of CTPht neat and other products that do not contribute to BaP air levels. The following works are performed and might have the potential for exposure:

- „A-Seite“ (or “laboratory BA”), n = 5, day shift only (8 h/day, 5 days/week)
    - Performing standard analytics - performed on each sample provided from production facility, thus exposure to CTPht/oil and CTP/AO formulations occurs dependent of relative amount of these formulations on the total production volume → i.e. currently **< 5% of their yearly working time** (but potentially up to 8 hours during their shift) [redacted]
- „C-Seite”, n = 7, night and late shift (8 h/day, 5 days/week)
    - **< 5% of their yearly working time**, up to 1 hour per shift
- 3rd section: additional laboratory workers, n= 3 on day shift (8 h/day, 5 days/week)
    - **< 5% of their yearly working time**, up to 1 hour per shift

Thus there is a total of 15 laboratory workers performing analysis with CTPht containing formulations.

Work takes place in the fume cupboard. Sample preparation in case of solid test material is in a closed mill with suction. All laboratory workers wear gloves according to the glove plan and required PPE (safety googles, work clothing). In case of recovery of solid samples a dust mask is worn.

Any waste is disposed in the so-called pitch container, which goes into waste intermediate storage (AZL) and is subsequently disposed of (incineration).

Description of data used for assessment of workers' exposure

Inhalation exposure

<u>Air measurements:</u>

Some personal samples (air measurements) are already available at RÜTGERS Germany, from samples taken between 2011 and 2015.

Table 9-54: Exposure concentrations of benzo[a]pyrene from personal air sampling (years 2011 to 2015)

Date	Activity	Measured concentration [µg/m³]	Measuring period [h]	Measuring period [min]	Exposure period [h/shift]	Exposure shift mean [µg/m³ per 8h]
07.09.2011 [a]	Routineanalytik, Raum 0.1, 0.2, 0.3	0.16	5.35	321	6.0	0.12
07.09.2011 [a]	Spezialanalytik, Raum 1.1, 1.2, 1.6	0.16	5.35	321	6.0	0.12
30.07.2013 [a]	Spezialanalytik, Raum 1.1, 1.2, 1.6	0.016	5.35	321	6.0	0.012
15.09.2015 [b]	Spezialanalytik, Raum 1.1, 1.2	<0.02	5.27	316	6.0	<0.02
15.09.2015 [b]	Prozessoptimierung, Raum 2.1, 2.2, 2.6	1.0	1.07	64	6.0	0.75

[a] method of determination: PAS-Langzeit/NIOSH 5506; [b] method of determination: PAS-Langzeit/NIOSH 5515

Remarks on exposure data:

From years 2011 to 2015 some (personal) air monitoring data are available. Concentrations ranged from below 10 ng/m^3 BaP to 750 ng/m^3 BaP. As explained above, reconstruction of the laboratory is planned.

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 exposure data, but – based on this exemption – refrain from calculating excess cancer risks for this contributing scenario.

9.1.8 Worker contributing scenario 6 – PROC 28 – Maintenance workers

9.1.8.1 Conditions of use

Table 9-55: Conditions of use

Product (Article) characteristics
• Percentage (w/w) of substance in mixture:> 50 - < 80% CTPht • Physical form of the used product: solid
Amount used (or contained in articles), frequency and duration of use/exposure
• Duration of activity: ≤ 8 h/day
Technical and organisational conditions and measures
• ABF-licence system before maintenance/cleaning operations • Emptying of lines before opening
Conditions and measures related to personal protection, hygiene and health evaluation
• Dermal protection: Yes • Respiratory Protection: Yes • Other PPE: standard safety equipment (Chemical protection suit Microchem 4000, safety shoes, helmet with face shield or goggles)
Other conditions affecting workers exposure
• Place of use: Outdoor • Operating temperature: ≤ 30°C (in tasks related to potential exposure)

9.1.8.2 Exposure and risks for workers

<u>RÜTGERS Germany maintenance workers:</u>

There are a total of 60 maintenance workers (total yearly working time: 60 workers x 220 days x 8 h/day = 105 600 h). Basically, maintenance work is always carried out with a valid work permit (ABF-licence system, see also 9.1.1.4). The work will take place only after approval by the company. Before starting work, the production responsible personnel determines which particular PPE must be worn on the basis of possible hazards. In general, the maintenance employees always wear the standard PPE on-site (helmet, goggles, gloves, safety shoes, work clothes).

In addition, when performing maintenance works the following PPE is applicable:

- Chemical protection suit Microchem 4000
- Respirator with ABEK filter or Respirator with hose
- Protective gloves according to glove plan or specification via ABF certificate
- goggles, helmet, work suit, safety shoes S3, face shield etc.

According to operation instructions (“BA-IH-32_Tragezeitbegrenzung_Atemschutzmaske _Chemikalienschutzanzug JBL”) the maximum wearing time for e.g. Full mask with filter with fan support and chemical protection suit is 120 minutes followed by a resting time of 30 minutes and maximum 3 times per shift.

Most maintenance cases are assigned to the tar refinery/manufacture processes. At the PÖ-Mix/Ölbetrieb facility each day on average one maintenance job is performed and around 2 to 4 maintenance workers are involved (usually only Monday until Friday). These maintenance jobs related to CTPht mixtures and potentially leading to exposure may occur on pumps, valves, loading pipes/arms, however as mentioned above stringent procedures apply regarding cleaning and flushing prior to maintenance. In case of cleaning activities, 2 maintenance workers are opening the lines (only after complete emptying beforehand) for 4 external workers who then carry out the cleaning tasks (described below). Only for a limited time during the year these facilities hold formulations relevant for this AfA, but this might increase in the future ([redacted] (20-100)%). On basis of the very different tasks performed by the maintenance workers estimation of time close to the PÖ-Mix/Ölbetrieb tanks or the dedicated filling stations is difficult. Task durations vary from a few minutes to whole shift length (for later consideration an average task duration of 4 h is assumed). There are also tasks with no exposure, e.g. scaffolding and insulation.

Based on the above described conditions the following working time is assumed: 2 to 4 maintenance workers perform any kind of repair on 220 days of the year with average task duration of 4 hours. In total this yields 1 760 to 3 520 h (i.e. 3.5 to 7.5 working days per year per worker). However when comparing the amount of CTPht used for mixtures relevant for this AfA to the total amount of CTPht produced, this amount accounts for [redacted] (20-100)% only. Thus [redacted] (the respective amount) of the working time calculated for maintenance workers is assumed to be related to tasks with CTPht mixtures in the future (i.e. approx. [redacted] (1.5-7.5) working days per year per worker).

<u>Contractors from external companies:</u>

Specialised contractors with special cleaning equipment hose out the loading pipes with e.g. high-pressure water jet technology, and absorb the emerging wastewater. The specialised chemistry vacuum truck used for these activities is operated by two workers. One tank truck loading site is cleaned every 4 weeks; all other loading stations are cleaned only when necessary. Tank cleaning is performed only if necessary as it is associated with immense efforts. For a conservative assumption one tank cleaning is included for estimation of workload. As mentioned above only for a limited time during the year all of these facilities hold formulations relevant for this AfA, which might increase in the future up to [redacted] (20-100)%. In addition, in case there is any spillage at any of the relevant facilities these external maintenance workers will perform the cleaning. Workers are using adequate personal protective equipment.

Based on the above described conditions the following working time is assumed:

- 4-weekly cleaning of one loading site — 13 times x 8 h x 4 workers = 416 h
- Cleaning on demand for other loading sites — 6 times x 8 h x 2 workers = 96 h
- Cleaning of tanks when necessary — 1 times x 16 h x 2 workers = 32 h
- Occasional cleaning of spills — 5 times x 4 h x 2 workers = 40 h

For all of these tasks the total working time is summed up to be approximately 600 h. As described above, when comparing the amount of CTPht used for mixtures relevant for this AfA to the total amount of CTPht produced, this amounts accounts for up to [redacted](20-100)% in the future. Thus [redacted] (the respective amount) of the working time from external maintenance workers is assumed to be related to tasks with CTPht mixtures (i.e. [redacted] (120-600) h).

Description of data used for assessment of workers' exposure

Inhalation exposure

Air measurements:

Some personal samples (air measurements) are available at RÜTGERS Germany. There are two samples form the mechanical workshop when welding was performed.

Table 9-56: Exposure concentrations of benzo[a]pyrene from personal air sampling (year 2015; method of determination: PAS-Langzeit/NIOSH 5506)

Date	Activity	Measuring period [h]	Measuring period [min]	Exposure period [h/shift]	Exposure [mg/m3]
05.05.2015	Welding	0.30	18	4.0	0.001
05.05.2015	Welding	0.28	17	4.0	0.001

In addition to this air sampling a biomonitoring campaign was performed recently. Samples were taken also from RÜTGERS Germany maintenance workers in September 2018. All raw data are presented in separate file in IUCLID section 13. Further details are provided in Annex XII – Biomonitoring Campaign.

For maintenance, samples were taken from workers after finishing a task with possible exposure (no further information on the tasks performed available). Importantly, all samples were taken contamination free. This means that specimen collection was performed after taking off the work clothes and washing hands or showering at the end of the activities involved. Collection was carried out directly in the urine cup.

There are a total of 60 RÜTGERS Germany Maintenance workers. During the biomonitoring campaign in three occasions samples were taken from two volunteers. They were both non-smokers (see Table 9-57).

Table 9-57: Results from biomonitoring campaign of 2 RÜTGERS Germany maintenance workers in September 2018; values are given as 1-hydroxypyrene in urine (µg 1-OHP/g creatinine), measured after end of task

	# of operators	# of measurements	arithm. mean	max	90th percentile
total	2	3	0.55	0.80	0.73
smoker	0	0			
non-smoker	2	3	0.55	0.80	0.73

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 (BaP conc.) the equation as given in ECHA (2018) is used:

$$\mathbf{BaP\ conc.}\,[\mathbf{ng/m^3}] = \frac{(\mathbf{1\text{–}\ OHP\ urinary\ concentration}\ \ [\mathbf{\mu mol/mol\ creatinine}] - \mathbf{1.13})}{\mathbf{11.1}}$$

In the following table 90th percentile values for the two different groups of workers as shown in Table 9-58 are converted into BaP air concentrations.

Table 9-58: 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)
Maintenance worker	0.73	0.38	-

No excess risks are calculated for maintenance workers. Their exposure levels are low and thus their 1-OHP levels are below 1.13 µmol/mol creatinine (90th percentile 0.38 µmol/mol creatinine), it can be reasonably assumed that their exposure is not far from background exposure levels.

<u>Contractors from external companies</u>

Contractors from external companies will work on the RÜTGERS Germany site. However, only a fraction of these workers are dedicated to work in facilities in the northern area relevant for this AfA. In addition, also the amount of time activities have to be performed and are related to the relevant formulations is limited.

There are no air measurements or biomonitoring data available for the external maintenance workers. However based on the above presented considerations on the working time spent with activities related CTPht mixtures relevant in this AfA a qualitative estimation can be provided.

The overall working time for relevant tasks of maintenance workers from RÜTGERS Germany was calculated to vary between [redacted] (1.5-7.5) working days per year per worker. With the biomonitoring data at hand no excess risks were calculated as the measured exposure was low.

The overall working time for external maintenance workers is around [redacted] (120-600) hours, thus being at the lower end compared to the maintenance workers from RÜTGERS Germany. As described above for all maintenance workers (i.e. external and RÜTGERS Germany workers) the same strict protocols apply for procedures to be performed and PPE to be worn, thus external maintenance workers are assumed to be exposed in the same order of magnitude as workers from RÜGERS Germany. In conclusion, as the working time is around the same for external maintenance workers also no excess risk is calculated as the exposure is considered to be as low as measured for RÜTGERS Germany maintenance (see Table 9-58).

Dermal exposure

As explained above, for most activities dermal exposure is not possible, as the material are kept at temperatures as high as [redacted]°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 handled on-site or are delivered to the repair shop are thoroughly drained before repair. Therefore, only residual contaminations remain on the objects. Contamination of surfaces would also be readily detected due to the black colour of all materials containing coal tar pitch. Maintenance workers 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, the following scenario is 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, 2003), 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[16]: activity performed one to three times per year per worker: 0.12 µg BaP/person/event * 3 events / 220 d/a = 1.63 ng BaP/person/day (under worst case assumptions with three events for each worker).

Comparison with uptake from inhalation at ambient background exposure concentrations

Total amount inhaled from background air exposure (mean of 0.321 ng BaP/m^3 measured in 2015 for sub-urban and urban regions, see Table 9-27) is calculated to be 6.42 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 4 compared to the amount taken up from inhaling ambient air with typical background concentrations of BaP (based on annual mean). 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 risks are

RÜTGERS Germany maintenance workers (n = 60): negligible

Contractors from specialised company (n unkown, however there are 2 workers on each chemistry vacuum truck): negligible

[16] Maintenance services EPT/PÖ-Mix and Ölbetrieb in 220 cases with 2 to 4 workers, total of 440 to 880 cases for 60 workers. Only 1/6 of the cases potentially related to handling of contaminated objects (i.e.74 to 147 cases), thus activity one to three times per year per worker. (Please note: in 2018 there were approximately 60 cases of repairs with potential for exposure, thus general assumptions above taken for comparison are thus considered conservative.)

10 RISK CHARACTERISATION RELATED TO COMBINED EXPOSURE

10.1 Human health (related to combined exposure)

10.1.1 Workers

The WCS for the use 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 for each activity. No combined exposure from different WCS occurs.

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 central Germany.

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 PLAN

Figure 12-1: Site plan of RÜTGERS Germany GmbH, Kekuléstr. 30, Castrop-Rauxel, North Rhine-Westphalia, Germany

Figure 12-2: Enlarged northern area with relevant facilities of the RÜTGERS Germany GmbH production site

13 ANNEX II – DETAILS ON EXHAUST GAS COMBUSTION FACILITIES

Plant certificate with limit values

Anfragespezifikation AVS 3 & REA Anhang 6 Grenzwertliste		
WY 10 1027	22. Oktober 2010	Seite 1 von 1

weyer gruppe

Grenzwertliste

Parameter	TA Luft 2002 Tagesmittelwert [1)]
Stickstoffoxide	≤ 350 mg/m³
Staub	≤ 20 mg/m³
Gesamtkohlenstoff	≤ 50 mg/m³
Kohlenmonoxid	≤ 100 mg/m³
Ammoniak	≤ 30 mg/m³
Quecksilber	< 0,05 mg/m³
Schwefeldioxid und Schwefeltrioxid als Schwefeldioxid[2)]	≤ 350 mg/m³
Bemerkungen	Alle Werte gelten bezogen auf das Reingasvolumen im Normzustand bei einem Betriebssauerstoffgehalt (273 k, 1.013 hPa nach Abzug des Feuchtegehaltes an Wasserdampf, angenommen wird ein O_2-Gehalt von 11 %) inklusive aller An- und Abfahrvorgänge der Anlage. Die o.g. genannten Grenzwerte liegen in der ersten Teilgenehmigung bereits vor.

1) Die Halbstundenmittelwerte betragen das Doppelte der Tagesmittelwerte

2) Der SO_3-Gehalt der Rauchgase der TNVs darf durch die REA ohne die Option eines Nasselektrofilters nicht erhöht werden

Für oben nicht genannte Parameter sind grundsätzlich die Grenzwerte nach TA Luft einzuhalten, die Anlage wird nach 4. BImschV Ziff. 1.2 Spalte 2 genehmigt werden.

Flue gas combustion data / inlet flue gas desulphurisation unit (REA)

Rauchgasdaten Abgasverbrennung / Eintritt REA

Es gibt zwei Abgasverbrennungsaggregate (AVS 1 und AVS 3), die parallel betrieben werden können und folglich beide in eine Entschwefelungs-anlage einspeisen können.

Rauchgasparameter

		AVS 1		AVS 3	
		von	bis	von	bis
Mengenstrom	Nm^3/h	5.000	6.500	10.000	13.500
Temperatur	°C	270	290	300	330
Druck	mbar ü	*	*	*	*

* Beide Abgasverbrennungsaggregate besitzen jeweils ein Saugzuggebläse, dass auf den Brennkammereintrittdruck geregelt ist. Der Austrittdruck ist der Druck am Eintritt in den Kamin. Die derzeit vorhandene, nicht betriebsbereite REA besitzt daher ein eigenes Saugzuggebläse. Mit dieser Konfiguration und Auslegung sind vermutlich nur kleine Überdücke von wenigen mbar am Eintritt in eine mobile REA zu realisieren.

Rauchgaszusammensetzung

		von	bis	Bemerkung
Sauerstoff (O2)	Vol. %	9	12	im Teillastbetrieb auch höher
Feuchte	g/m^3	80	110	
Feuchte	Vol. %	9	12	
Kohlendioxid CO2	Vol. %	5	7	
Schwefeldioxid (SO2)	mg/m^3	2.500	6.300	
Schwefeltrioxid (SO3)	mg/m^3	100	250	bei 5.000 - 6.000 N/m^3 (nur AVS 1) - Die Fracht wird nicht größer, wenn beide Aggregate laufen.
Quecksilber	mg/m^3	0,04	0,25	
Stickoxide (NO+NO2)	mg/m^3	200	850	bis 300 mg/Nm^3 thermisches NOx, bis zu 500 N/m^3 aus Brennstoffstickstoff
Gesamtstaub	mg/m^3	0,5	5	Hauptbestandteile Ca- und Zn-Verbindungen

14 ANNEX III – WASTE DISPOSAL NOTIFICATIONS

Examples of on-site documentation for waste disposal proof. The documented waste is not associated with the formulation process.

Abfall	RÜTGERS Matrerialnummer	Abfall-schlüssel-nummer	aktueller Entsorgungs-nachweis	Entsorger			Entsorgungsanlage			Entsorgungsverfahren nach Anhang 1 & 2 KWG	
kontaminuiertes Holz	EV120747 Altholz (A4)	170204	ENE1RRG00664	RRG Rheinische Recycling GmbH	Elkanweg	41748 Viersen	RRG Entsorgungs-anlage	Elkanweg	41748 Viersen	sonstiges Verfahren	R12
kontaminuiertes Holz	EV120747 Altholz (A4)	170204	ENE9U100300	BMK-Biomassekraftwerk Lünen GmbH	Josef-Rethmann-Straße	44536 Lünen	Altholz-aufbereitung	Brunnenstraße	44536 Lünen	sonstiges Verfahren	R12
kontaminuierter Dämmstoff	EV120742 Dämmaterial aus Baumaßnahmen	170603	ENE5G0202055	AGR Abfallentsorgungs-Gesellschaft Ruhrgebiet mbH	Im Emscherbruch	45699 Herten	Asbest Mono Bereich	Wiedehopfstr.	45892 Gelsenkirchen	oberirdische Deponie	D01
kontaminuierter Dämmstoff	EV120742 Glaswolle stark verschmutzt	170603	ENE5G0202315	AGR Abfallentsorgungs-Gesellschaft Ruhrgebiet mbH	Im Emscherbruch	45699 Herten	Asbest Mono Bereich	Wiedehopfstr.	45892 Gelsenkirchen	oberirdische Deponie	D01
Abfallpech	EV120111 Abfallpech	050603	ENE5R1904383	AGR Abfallentsorgungs-Gesellschaft Ruhrgebiet mbH	Im Emscherbruch	45699 Herten	IM-Line	Im Emscherbruch	45699 Herten	Thermische Behandlung	R01
Teerhaltiger Abfall	EV120701 Dreiphasendekanter-feststoff	050603	ENE5R1903723	AGR Abfallentsorgungs-Gesellschaft Ruhrgebiet mbH	Im Emscherbruch	45699 Herten	IM-Line	Im Emscherbruch	45699 Herten	Thermische Behandlung	R01
kontaminierer Schrott	EV120768 verunreinigter Schrott	170409	ENE1RRG00452	RRG Rheinische Recycling GmbH	Elkanweg	41748 Viersen	RRG Entsorgung-sanlage	Elkanweg	41748 Viersen	sonstiges Verfahren	R04
Laborchemikalien	Sammelentsorgung	160506	SNE1MGX01741	REMONDIS Industrie service GmbH&Co KG	Brunnenstrasse	44536 Lünen	REMONDIS Niederlassung Mühlheim	Pilgerstraße	45473 Mühlheim	sonstiges Verfahren	D13
Lösungsmittel	Sammelentsorgung	140603	SNE3MYC00109	REMONDIS Industrie service GmbH&Co KG	Brunnenstrasse	44536 Lünen	Zwischenlager und CPB	Am alten Bahnhof	51645 Gummersbach	sonstiges Verfahren	R13
Lösungsmittel, wasserhaltig	Sammelentsorgung	070104	SNE3MYC00104	REMONDIS Industrie service GmbH&Co KG	Brunnenstrasse	44536 Lünen	Zwischenlager und CPB	Am alten Bahnhof	51645 Gummersbach	sonstiges Verfahren	R13
kontam. Metallemballagen	Sammelentsorgung	150110	SNE1MHX00397	GMVA Neiderrhien GmbH	Liricher Straße	46049 Oberhausen	GMVA Neider-rhein GmbH	Buschausener Str.	46049 Oberhausen	Thermische Behandlung	R01
kontam. Metallemballagen	Sammelentsorgung	150110	SNE5B1400109	Fa. Bernhard Sandkuhle	Klendergarten	48683 Ahaus	Metall-aufbereitungs-anlage	Heeker Straße	48683 Ahaus	Chemisch-/physikalische Behandlung	R04

This documentation as to be performed according to the German Waste Management Act ("Kreislaufwirtschaftsgesetz", KrWG). Therein also the explanations for the disposal procedures mentioned as abbreviations above are explained (as only German documentation is available no further texts are annexed, but can be looked up at respective German Federal Ministry http://www.gesetze-im-internet.de/krwg/index.html).

15 ANNEX IV – PHOTO DOCUMENTATION – SAMPLING

Figure 15-1 Sampling point CF90 (including exhaust ventilation) - Visual inspection

Figure 15-2 CF90 - Worker opening substance flow

Figure 15-3 CF 90 - Worker closing lid of sampling vessel

Figure 15-4 Opening closed sampling point #A (no exhaust ventilation)

 **Figure 15-5 #A Installation of sampling vessel**	 **Figure 15-6 #A opening substance flow and visual inspection of filling**
 **Figure 15-7 #A Removal of sampling vessel**	 **Figure 15-8 #A Closing sampling vessel**

Figure 15-9 Opening closed sampling point #B (no exhaust ventilation)

Figure 15-10 #B opening substance flow and visual inspection of filling

Figure 15-11 #B Removal of sampling vessel - 1

Figure 15-12 #B Removal of sampling vessel - 2

16 ANNEX V – PHOTO DOCUMENTATION – LOADING PÖ-MIX

Figure 16-1 Worker opening manhole - 1

Figure 16-2 Worker opening manhole - 2

Figure 16-3 Worker opening manhole - 3

Figure 16-4 Worker removing drainer before loading

Figure 16-5 Worker starting automated movement of loading arm - 1

Figure 16-6 Worker starting automated movement of loading arm - 2

Figure 16-7 Loading arm placed on top of manhole

Figure 16-8 Loading arm final placement

Figure 16-9 Worker operating loading arm after loading completed

Figure 16-10 Worker operating loading arm after loading completed

Figure 16-11 Photo documentation according to ADR*

* After loading is completed a photo of the lid is made for the ADR (transport of dangerous goods regulations) documentation to document that everything was closed and unpolluted at the time the truck left the factory. The camera is operated without glove.

17 ANNEX VI – PHOTO DOCUMENTATION – ON-SITE ANALYTICS

Figure 17-1

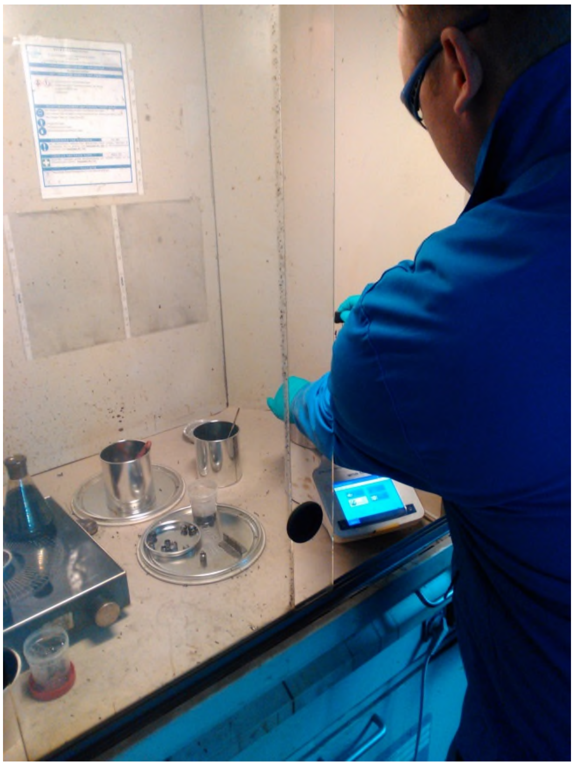
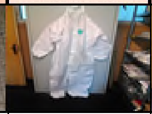
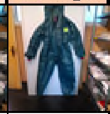
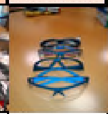
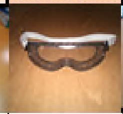
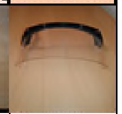


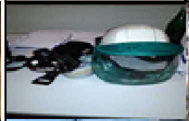
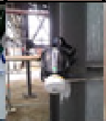
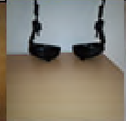
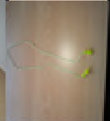
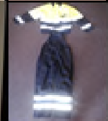
Figure 17-2

Worker during on-site analysis in the dedicated lab room of the central control room for PÖ-Mix facility

18 ANNEX VII – DETAILED OVERVIEW OF PPE AVAILABLE INCLUDING STANDARDS COMPLIED WITH

Relevant for the uses in this AfA are “Verladung Nord” (loading stations in the northern part of the site); “Zentrale Messwarte” (central control room), and “Zentrallabor” (central laboratory for analysis)

PSA	Schutzhelm	Arbeitsanzug	nistatische Schutzkleidur	Kittel	Overall weiss	Overall grün	Schutzbrille	orbschutzbril	Visier lang	Visier norma
"Probenahme										
			Zum Schutz gegen Regen, für				diverse			für MSA
			hitzeschutzexponierte Arbeiter							V-Gard 5000
			u. gegen flüssige Chemikalien							
			"Phenolschutzanzug"							
TYP	MSA V-Gard	3 Punkt		Baumwoll	Microgard 2000	Micogard 4	UVEX	3 M	MSA	Sordin 1
		Multi Proof	Ötscher Seriennummer 7852						ITM/NOSOR	
									60042	
				zukünftig						
Norm	EN 397	EN ISO 11611	EN ISO 20471:2015 A1 B!2	EN ISO 116	Type 5 EN ISO 1	Typ 3 EN 14	DIN EN 166	DIN EN 166	DIN EN 16	EN 166: 1995
		EN ISO 11612	EN 1149-3:2004		Type 6 EN13034	Typ 4 EN 14605				
		EN 61482-1-2	EN 13034:2009 Typ 6		EN14126	Typ 5 EN ISO				
		EN 13034 Ty	EN 343:2010 Klasse 3/3		EN1073-2	EN 14126				
		EN 1149-3			EN1149-5	EN 1073-2				
		EN 1149-5			DIN 32781	EN1149-5				
Verladung Nord	x	x			bei Bedarf	bei Bedarf	x	x		x
Verladung C-Betrieb	x		x		bei Bedarf	bei Bedarf	x	x		x
Absackung	x	x			x	bei Bedarf	x	x		x
Naphthalinbetrieb	x	x			bei Bedarf	bei Bedarf	x	x		x
Zentrale Messwarte I	x	x			bei Bedarf	bei Bedarf	x	x		x
Zentrallabor		nur Hose		x	bei Bedarf		x	x		x
Werkstätten	x	x			bei Bedarf	bei Bedarf	x	x		x
KTD-Messwarte	x	x			bei Bedarf	bei Bedarf	x	x		x

PSA	Atemschutzmaske	Maske	Staubfilte	Arbeitsschuh	Gehörschutz	Gehörschutz	ehörschut	Regenjack	rbeitshandschu	Arbeitshandschu	beitshandsch	rbeitshandschu
*Probenahme	 											
									Leder	Unterhandschuh	Chemie	Mechanik
										grün und blau	grün	gelb
TYP	PM u. Scott Prowf	BRK 730	3 M	UVEX S 3	Sealed Air	MSA Mediu	UVEX	Sioen	V+R Seiz	Ansell TNT 92/(	Ansell Alpha T	KCL Honeywell
	mit div. Atemanschlüssen		Aura FF P2		UVEX etc.						58-535	
			9322 u FF									
			P3 8835+									
Norm	ATEX 95	EN 136	EN 149:20	EN ISO 2034	EN 352	EN 352 Type	EN 352	EN 340	EN 388	EN 420	EN 374	EN 388
	ATEX 137	Kl. 2	A1:2009					EN 531:1995		EN 374-1-3		
	EN 12941	EN 148-1						EN 1149-5				
	EN 12942							EN ISO 14116				
								EN 471				
								EN 343				
Verladung Nord	x	x	b. Bed.	x		x	x	bei Bedarf	x	x	x	x
Verladung C-Betrieb		x	b. Bed.	x		x	x	bei Bedarf	x	x	x	x
Absackung		x	x	x		x	x	bei Bedarf	x	x	x	x
Naphthalinbetrieb	x		b. Bed.	x		x	x	bei Bedarf	x	x	x	x
Zentrale Messwarte I	x	x	b. Bed.	x		x	x	bei Bedarf	x	x	x	x
Zentrallabor			b. Bed.	x		x	x	bei Bedarf	³siehe unten	³siehe unten	³siehe unten	³siehe unten
Verkstätten	x	x	x			x	x	bei Bedarf	x	x	x	x
KTD-Messwarte	x	x	b. Bed.	x		x	x	bei Bedarf	x	x	x	x

* Employees of the central laboratory use the following gloves: MicroFlex and TuchNTuff. Heat protection u. Cold protection gloves will be introduced
2 As a substitute (for our safety): Nomex Comfort consists of 93% Meta-Aramid Nomex, 5% para-Aramid Kevlar, 2% "Kohlemantelfaser" P140, Application: Industry EN ISO 11612
3 For sampling of the above mentioned areas the following gloves are to be worn: For tar-based products, underglove + leather glove, for oil-based products and chemicals

19 ANNEX VIII – BREAKTHROUGH TIMES ACCORDING TO RÜTGERS GERMANY GLOVE PLAN

Table 19-1: Breakthrough time [minutes] according to glove plan

Glove Type **Substance**	**Ansell AlphaTec 58-535 (nitrile)**	**Sol-Vex Premium 37-900 (nitrile)**	**Barrier 02-100 (Laminate film (polyethylene nylon))**	**ChemTek 38-628 (Viton / Butyl)**	**Touch N Tuff 92-600 (nitrile)**
AO (CAS 90640-80-5)	> 480	> 480	> 480	> 480	60-120
CTPht (CAS 65996-93-2)	> 480	> 480	> 480	> 480	> 480

The given breakthrough times according to EN374-3:2003 in minutes are corresponding to Category 3 medium protection for the Touch N Tuff 92-600 (nitrile) glove when working with AO containing mixtures. However all other gloves provide the highest protection level possible (> 480 minutes, Category 6).

20 ANNEX IX – PAH DRAINAGE AFTER BIOLOGICAL TREATMENT PLANT

There are several measurements available for measurements of individual PAHs in the effluent of the on-site biological WWTP. Relevant PAHs for environmental assessment are marked in grey in the table below. From these 71 measurements in years 2015 to 2017 mean value of all PAH is 70.1 µg/L. The drainage after the biological treatment plant is quite variable, with a minimum sum value of 1.0 µg/L and a maximum value of 983.2 µg/L.

Table 20-1: PAH measurements[a] after biological treatment plant

		Sum PAH	Naphthalene	Acenaphthene	Fluorene	Phenanthrene	Anthracene	Fluoranthene	Pyrene	Benz[a]-anthracene	Chrysene	Benzo[b]-fluoranthene	Benzo[k]-fluoranthene	Benzo[a]-pyrene	Dibenzo[ah]-anthracene	Benzo[ghi]-perylene	Indeno[1,2,3-cd]-pyrene
Date	Day	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L	µg/L
05.01.2015	Mon	25.98	4.82	0.4	0.52	6.68	0.22	2.76	1.89	0.8	1.16	1.01	0.46	1.09	0.04	2.79	1.34
19.01.2015	Mon	7.07	3.16	0.27	0.15	0.81	0.06	1.06	0.69	0.07	0.23	0.08	0.05	0.08	0.07	0.29	<0.1
04.02.2015	Wed	20.8	13.18	0.94	0.24	0.92	0.63	1.67	1.16	0.2	0.27	0.39	0.18	0.4	0.01	0.27	0.34
04.03.2015	Wed	5.64	1.23	0.39	0.41	1.03	0.37	1	0.68	0.06	0.13	0.09	0.04	0.07	0.01	0.06	0.07
16.03.2015	Mon	52.06	16.4	1.76	2.16	5.9	2.54	9.19	5.61	0.75	1.66	1.81	0.81	1.29	0.12	0.89	1.17
13.04.2015	Mon	26.35	17.54	0.45	0.08	1.78	0.83	2	1.27	0.27	0.46	0.43	0.18	0.36	0.05	0.3	0.35
11.05.2015	Mon	27.9	21.4	0.51	1.1	1.16	0.74	0.12	2.03	0.04	0.02	0.02	0.01	0.32	0.1	0.04	0.29
28.05.2015	Thurs	8.08	0.54	0.25	0.08	0.53	0.88	2.78	1.7	0.18	0.38	0.19	0.09	0.15	0.02	0.15	0.16
08.06.2015	Mon	3.07	0.74	0.17	0.07	0.34	0.01	0.86	0.52	0.06	0.02	0.06	0.04	0.05	0.01	0.06	0.06
22.06.2015	Mon	4.26	0.6	0.16	0.05	0.32	0.02	0.68	0.48	0.02	0.17	0.56	0.23	0.45	0.03	0.2	0.29
01.07.2015	Wed	2.97	0.82	0.21	0.07	0.37	<0.01	0.43	0.44	0.04	0.02	0.16	0.08	0.16	0.01	0.09	0.07
13.07.2015	Mon	8.63	1.04	0.18	0.07	0.4	1.06	3.57	0.07	0.05	0.14	0.79	0.27	0.21	0.03	0.32	0.43
28.07.2015	Tue	38.51	3.74	0.73	6.87	3.04	0.33	7.12	5.81	1.08	0.72	2.82	1.29	2.21	0.14	1.26	1.35
10.08.2015	Mon	4.04	0.88	0.37	0.31	0.55	0.63	0.51	0.36	0.08	0.04	0.09	0.03	0.05	0.01	0.05	0.08

25.08.2015	Tue	7.42	0.5	0.45	0.33	0.72	1.11	0.43	0.47	0.07	0.03	0.83	0.35	0.81	0.05	0.61	0.66
07.09.2015	Mon	72.93	54.49	7.5	1.54	2.05	2.11	1.95	1.7	0.24	0.1	0.4	0.19	0.37	0.01	0.14	0.14
07.10.2015	Wed	4.07	1.1	0.16	0.08	0.55	0.02	0.53	0.52	0.1	0.2	0.25	0.11	0.21	0.02	0.13	0.09
27.10.2015	Tue	1.51	0.41	0.04	0.02	0.15	0.01	0.14	0.15	0.02	0.05	0.05	0.02	0.05	0.01	0.04	0.35
24.11.2015	Tue	10.1	1	0.48	0.94	4.96	0.33	0.2	1.41	0.04	0.1	0.1	0.05	0.12	0.02	0.18	0.17
08.12.2015	Tue	3.91	1.08	0.22	0.2	0.9	0.07	0.51	0.4	0.07	0.12	0.09	0.04	0.07	0.01	0.07	0.06
21.12.2015	Mon	11.21	8.49	0.27	0.18	0.68	0.02	0.22	0.25	0.08	0.13	0.18	0.08	0.2	0.02	0.19	0.22
04.01.2016	Mon	9.01	0.21	0.32	0.28	2	0.26	0.17	2	0.31	0.1	1.15	0.52	1.05	0.04	0.29	0.31
18.01.2016	Mon	21.4	3.53	0.22	0.72	7.31	0.3	3.52	2.04	0.24	0.59	0.87	0.43	0.77	0.05	0.38	0.43
02.02.2016	Tue	7.83	1.45	0.27	0.08	0.47	0.03	1.29	1.05	0.23	0.47	0.66	0.32	0.59	0.06	0.42	0.44
17.02.2016	Wed	536.49	206.8	85.1	43	74.1	7.2	75.2	35.3	2.6	3.5	1.3	0.6	1.1	0.05	0.3	0.34
08.03.2016	Tue	302.48	18.51	98.18	19.46	2.87	7.85	93.4	46.51	3.89	4.57	2.22	1.2	2.09	0.11	0.7	0.92
23.03.2016	Wed	172.22	11.88	14	0.31	2.87	1.99	92.6	32.8	4.29	4.79	2.36	1.26	1.39	0.13	0.72	0.83
05.04.2016	Tue	111.98	8.8	6.72	5.06	28.1	11.27	27.6	14.7	0.37	0.89	2.9	1.26	2.45	0.12	0.87	0.87
18.04.2016	Mon	23.42	1.52	0.19	0.15	0.42	0.27	8	4.75	0.54	1.01	1.9	0.98	1.4	0.15	1.04	1.1
02.05.2016	Mon	6.23	1.26	0.13	0.05	0.47	0.06	0.39	0.58	0.14	0.32	0.85	0.42	0.85	0.03	0.31	0.37
18.05.2016	Wed	4.3	0.72	0.14	0.05	0.3	0.02	0.88	0.57	0.03	0.07	0.33	0.12	0.27	0.05	0.35	0.4
30.05.2016	Mon	7.21	1.16	1.53	0.59	0.75	0.09	0.89	0.78	0.06	0.16	0.35	0.16	0.31	0.02	0.18	0.18
13.06.2016	Mon	11.9	2	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	2.9	1.1	2.8	<0.5	1.6	1.5
21.06.2016	Tue	23.14	4	0.61	0.27	0.63	0.95	0.75	1.95	0.11	0.95	6.07	1.71	2.71	0.15	1.15	1.13
04.07.2016	Mon	3.61	1.75	0.1	0.06	0.42	0.08	0.47	0.29	0.09	0.09	0.08	0.03	0.07	0.01	0.07	<0.01
18.07.2016	Mon	4.99	1.15	0.11	0.05	0.27	0.07	0.57	0.89	0.04	0.13	0.58	0.24	0.42	0.03	0.2	0.24
01.08.2016	Mon	11.6	6.02	0.55	0.24	1.01	0.1	0.5	0.67	0.07	0.19	0.8	0.33	0.64	0.03	0.23	0.22
08.08.2016	Mon	11.12	2.99	0.28	0.11	0.6	0.17	0.53	0.69	0.26	0.44	1.68	0.6	1.36	0.07	0.69	0.65
22.08.2016	Mon	1.014	0.33	0.04	0.04	0.1	0.01	0.09	0.074	0.01	0.04	0.07	0.03	0.07	0.01	0.05	0.05
05.09.2016	Mon	7.27	0.98	0.31	0.1	0.42	0.01	1.44	1.58	0.09	0.22	0.71	0.32	0.63	0.03	0.24	0.19
19.09.2016	Mon	273.05	3.76	1.01	0.62	56.2	5.37	128.25	66.92	1.08	2.22	3.12	1.13	1.44	0.42	0.88	0.63
04.10.2016	Tue	37.62	3.53	0.37	0.3	4.14	0.28	13.51	7.31	0.31	0.58	2.6	0.95	1.93	0.09	0.89	0.83

24.10.2016	Mon	6.83	0.3	0.65	0.11	0.49	0.13	0.87	0.72	0.24	0.54	1.04	0.34	0.69	0.03	0.34	0.34
07.11.2016	Mon	578.4	14.8	43.9	31.4	141.6	10.4	210.6	105.3	1.9	7.6	5.8	2	1.4	0.7	0.7	0.3
21.11.2016	Mon	53.85	3.5	1.04	0.33	3.3	0.61	26.5	13.63	0.23	0.45	1.83	0.48	1.03	0.04	0.45	0.43
05.12.2016	Mon	15.84	7.68	1.98	0.49	2.1	0.16	1.58	0.86	0.09	0.24	0.25	0.1	0.2	0.01	0.1	<0.1
27.12.2016	Tue	11.91	2.14	0.53	0.27	2.02	0.16	3.81	2.03	0.04	0.1	0.2	0.09	0.2	0.01	0.15	0.16
09.01.2017	Mon	164.24	5.11	1.02	0.43	21.51	2.49	84.23	33.79	0.77	1.66	6.17	1.7	2.86	0.13	1.14	1.23
23.01.2017	Mon	66.35	29.68	4.22	2.32	6.9	1.44	8.42	4.22	1.42	1.91	2.56	0.77	1.36	0.06	0.54	0.53
13.02.2017	Mon	14.9	8	0.17	0.09	0.72	0.38	1.26	0.16	0.47	0.51	0.95	0.4	0.85	0.08	0.38	0.48
27.02.2017	Mon	13.51	5.67	0.2	0.14	0.53	0.08	1.67	0.21	0.53	0.66	1.25	0.56	1.25	0.07	0.32	0.37
13.03.2017	Mon	59.2	32.9	9.7	4.38	0.1	0.76	6.45	0.06	0.46	0.6	1.17	0.58	1.04	0.07	0.42	0.51
27.03.2017	Mon	9.28	3.39	0.35	0.21	1.01	0.06	0.91	0.26	0.19	0.32	0.86	0.36	0.72	0.04	0.24	0.36
24.04.2017	Mon	14.28	5.45	0.4	0.24	0.93	0.18	1.09	1.16	1.11	0.41	1.03	0.45	0.88	0.05	0.32	0.58
08.05.2017	Mon	4.14	1.3	0.31	0.22	0.93	0.08	0.63	0.26	0.07	0.08	0.07	0.03	0.05	0.01	0.06	0.04
22.05.2017	Mon	5.74	0.87	0.27	0.14	0.01	0.11	1.55	0.74	0.14	0.15	0.48	0.19	0.46	0.04	0.27	0.32
07.06.2017	Wed	41.88	20.4	2.26	0.83	2.52	0.27	1.88	2.59	0.6	1.32	2.71	1.3	2.59	0.19	1.11	1.31
19.06.2017	Mon	5.07	1.35	0.19	0.13	0.45	0.03	0.26	0.1	0.03	0.15	0.77	0.3	0.68	0.04	0.3	0.29
03.07.2017	Mon	12.33	0.89	0.61	0.18	1.31	0.22	4.57	0.95	0.66	0.69	0.75	0.31	0.56	0.05	0.29	0.29
17.07.2017	Mon	11.46	2.54	2.04	0.34	0.98	0.2	1.2	1	0.2	0.42	0.15	0.5	0.91	0.07	0.44	0.47
31.07.2017	Mon	10.5	4	0.47	0.11	0.3	0.08	1.85	0.48	0.31	0.32	0.76	0.38	0.73	0.06	0.31	0.34
14.08.2017	Mon	73.91	7	4.4	3.7	21.6	1.4	21.4	7.8	1.1	0.97	1.01	0.61	1	0.13	0.87	0.92
28.08.2017	Mon	71.69	18.2	6.69	3.81	15.9	1.16	16.2	7.47	0.38	0.34	0.43	0.23	0.4	<0.05	0.23	0.25
11.09.2017	Mon	72.41	13.8	6.76	2.08	10.7	0.99	16.8	6.18	2.94	3.11	3.31	1.5	2.92	0.1	0.58	0.64
28.09.2017	Thurs	549.64	3.04	151	1.7	20.2	8.7	221	109	12.8	10.5	5.7	1.8	2.8	0.1	0.6	0.7
09.10.2017	Mon	983.2	168	196	73.8	303	37.1	118	63.8	7.5	6.5	3.9	1.5	2.6	0.1	0.6	0.8
23.10.2017	Mon	10.6	1.56	0.63	0.1	0.58	0.14	3.42	0.75	0.45	0.42	0.74	0.32	0.69	0.05	0.32	0.43
06.11.2017	Mon	27.57	1.95	0.63	0.11	0.47	0.06	7.3	3.66	0.22	1.07	3.56	1.67	3.57	0.21	1.36	1.73
20.11.2017	Mon	13.57	1	0.57	0.19	0.7	0.06	2.56	0.11	0.15	0.58	2.33	1.08	2.59	0	0.69	0.96
03.08.2018	Fri	60.3	9.5	4.1	0.7	1.7	0.6	4.9	4.2	0.8	1.7	12.4	3.3	7.7	1.7	3.2	3.8

20.08.2018	Mon	43.2	32.7	2.8	1	3	0.3	1.5	0.9	0.1	0.1	0.2	0.1	0.2	0.1	0.1	
17.09.2018	Mon	101.7	18	4.2	2	14	1.5	21.2	31.7	1.2	2	2.4	0.7	1.3	0.1	0.6	0.8
02.10.2018	Tue	260.4	152	67.7	14.5	18.1	3.3	0.3	1.8	0.2	0.2	0.7	0.3	0.7	0.1	0.3	0.2
05.11.2018	Mon	150.7	23.9	11.5	12.3	52.7	5.5	19.8	10.9	0.7	1.2	3.3	1.3	2.9	0.4	2	2.3
19.11.2018	Mon	69.5	6.2	5.2	0.4	1.7	1.2	29.4	13.7	1.9	2.5	2.6	1	2.2	0.2	0.7	0.6

Mon = Monday; Tue = Tuesday; Wed = Wednesday; Thurs = Thursday

[a] PAHs measured in wastewater at the RÜTGERS Germany GmbH laboratory according to DIN EN ISO 17993 with HPLC (fluorescence detection) after liquid-liquid extraction (limit of detection: 0.1µg/L or 0.1ppb).

21 ANNEX X – GERMAN FOOD CONSUMPTION, "NATIONALE VERZEHRSSTUDIE II"

Table 21-1: Consumption of the five EUSES food categories representative for the German population (MRI, 2008)

	Mean	Unit
Root crops		
Potatos	81	[g/day]
EUSES default for root crops	384	[g/day]
Consumption as % of default	21.09%	[%]
Leaf crops		
Vegetables	233	[g/day]
Cereals	276	[g/day]
Fruits	254	[g/day]
Sum	763	[g/day]
EUSES default for leaf crops	1200	[g/day]
Consumption as % of default	63.58%	[%]
Dairy products		
Milk and milk products, including cheese	254.5	[g/day]
EUSES default for dairy products	561	[g/day]
Consumption as % of default	45.37%	[%]
Meat		
Meat	121.5	[g/day]
Eggs	19	[g/day]
Fats	24.5	[g/day]
Sum	165	[g/day]
EUSES default for meat	301	[g/day]
Consumption as % of default	54.82%	[%]
Fish		
Fish	26	[g/day]
EUSES default for fish	115	[g/day]
Consumption as % of default	22.61%	[%]

Total consumption of all groups acc. to survey	1290	[g/day]
Total consumption of all groups acc. to EUSES	2561	[g/day]

22 ANNEX XI – EUSES PROTOCOLS FOR THE TEN RELEVANT PAHS

22.1 Anthracene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers 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	984C8059		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	0	[-]	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	2.10E-04	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	1.93E-10	[mg.l-1]	O
Regional PEC in seawater (total)	1.73E-11	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.84E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	1.70E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.34E-13	[mg.m-3]	O
Regional PEC in agricultural soil (total)	1.14E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	2.20E-13	[mg.l-1]	O
Regional PEC in natural soil (total)	1.32E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	1.32E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	2.31E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	2.05E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	4.03E-16	[mg.l-1]	O
Continental PEC in seawater (total)	6.77E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	3.85E-16	[mg.l-1]	O
Continental PEC in seawater (dissolved)	6.64E-15	[mg.l-1]	O
Continental PEC in air (total)	2.84E-16	[mg.m-3]	O
Continental PEC in agricultural soil (total)	2.43E-13	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	4.66E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	2.81E-13	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	2.81E-13	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	4.83E-13	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	8.02E-12	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	8.73E-16	[mg.l-1]	O
Moderate PEC in water (dissolved)	8.56E-16	[mg.l-1]	O
Moderate PEC in air (total)	1.25E-17	[mg.m-3]	O
Moderate PEC in soil (total)	1.23E-14	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	1.03E-12	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	6.57E-16	[mg.l-1]	O
Arctic PEC in water (dissolved)	6.44E-16	[mg.l-1]	O
Arctic PEC in air (total)	4.00E-18	[mg.m-3]	O

Arctic PEC in soil (total)	1.33E-14	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	7.79E-13	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	2.49E-16	[mg.l-1]	O
Tropic PEC in water (dissolved)	2.44E-16	[mg.l-1]	O
Tropic PEC in air (total)	7.01E-18	[mg.m-3]	O
Tropic PEC in soil (total)	3.65E-15	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	2.94E-13	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.741	[%]	O
Steady-state mass fraction in regional seawater	0.0739	[%]	O
Steady-state mass fraction in regional air	5.77E-03	[%]	O
Steady-state mass fraction in regional agricultural soil	0.997	[%]	O
Steady-state mass fraction in regional natural soil	0.13	[%]	O
Steady-state mass fraction in regional industrial soil	0.0481	[%]	O
Steady-state mass fraction in regional freshwater sediment	10.2	[%]	O
Steady-state mass fraction in regional seawater sediment	0.302	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.36E-04	[%]	O
Steady-state mass fraction in continental seawater	5.06	[%]	O
Steady-state mass fraction in continental air	2.12E-03	[%]	O
Steady-state mass fraction in continental agricultural soil	0.185	[%]	O
Steady-state mass fraction in continental natural soil	0.0241	[%]	O
Steady-state mass fraction in continental industrial soil	8.93E-03	[%]	O
Steady-state mass fraction in continental freshwater sediment	1.87E-03	[%]	O
Steady-state mass fraction in continental seawater sediment	1.03	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	36.3	[%]	O
Steady-state mass fraction in moderate air	1.04E-03	[%]	O
Steady-state mass fraction in moderate soil	0.0436	[%]	O
Steady-state mass fraction in moderate sediment	1.48	[%]	O

GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	17.9	[%]	O
Steady-state mass fraction in arctic air	1.81E-04	[%]	O
Steady-state mass fraction in arctic soil	0.0205	[%]	O
Steady-state mass fraction in arctic sediment	0.731	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	23.7	[%]	O
Steady-state mass fraction in tropic air	9.54E-04	[%]	O
Steady-state mass fraction in tropic soil	0.0127	[%]	O
Steady-state mass fraction in tropic sediment	0.966	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	6.94E-04	[kg]	O
Steady-state mass in regional seawater	6.92E-05	[kg]	O
Steady-state mass in regional air	5.40E-06	[kg]	O
Steady-state mass in regional agricultural soil	9.33E-04	[kg]	O
Steady-state mass in regional natural soil	1.22E-04	[kg]	O
Steady-state mass in regional industrial soil	4.50E-05	[kg]	O
Steady-state mass in regional freshwater sediment	9.56E-03	[kg]	O
Steady-state mass in regional seawater sediment	2.83E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	1.27E-07	[kg]	O
Steady-state mass in continental seawater	4.74E-03	[kg]	O
Steady-state mass in continental air	1.99E-06	[kg]	O
Steady-state mass in continental agricultural soil	1.73E-04	[kg]	O
Steady-state mass in continental natural soil	2.26E-05	[kg]	O
Steady-state mass in continental industrial soil	8.36E-06	[kg]	O
Steady-state mass in continental freshwater sediment	1.75E-06	[kg]	O
Steady-state mass in continental seawater sediment	9.68E-04	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.034	[kg]	O
Steady-state mass in moderate air	9.72E-07	[kg]	O
Steady-state mass in moderate soil	4.09E-05	[kg]	O
Steady-state mass in moderate sediment	1.39E-03	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0167	[kg]	O

Steady-state mass in arctic air	1.70E-07	[kg]	O
Steady-state mass in arctic soil	1.92E-05	[kg]	O
Steady-state mass in arctic sediment	6.85E-04	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0222	[kg]	O
Steady-state mass in tropic air	8.94E-07	[kg]	O
Steady-state mass in tropic soil	1.19E-05	[kg]	O
Steady-state mass in tropic sediment	9.05E-04	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	4.44E-10	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	6.42E-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)	6.42E-08	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.90E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	4.02E-09	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	4.02E-09	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.19E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	8.02E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	8.18E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.57E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.39E-11	[mg.l-1]	O
Local PEC in pore water of grassland	2.66E-11	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.39E-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	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	6.42E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	4.02E-05	[-]	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	6.77E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	4.24E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	6.37E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	1.84E-06	[-]	O
RCR for the regional marine compartment	1.70E-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	7.58E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	6.73E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	1.03E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

22.2 Phenanthrene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers 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	0A1C5B53		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	0	[-]	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	1.55E-03	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	1.47E-03	[ug.m-3]	O
Regional PEC in seawater (total)	1.30E-10	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.41E-09	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	1.28E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	3.07E-12	[mg.m-3]	O
Regional PEC in agricultural soil (total)	1.58E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	3.90E-12	[mg.l-1]	O
Regional PEC in natural soil (total)	1.80E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	1.80E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	1.37E-06	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	1.18E-07	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	2.12E-14	[mg.l-1]	O
Continental PEC in seawater (total)	5.36E-14	[mg.l-1]	O
Continental PEC in surface water (dissolved)	2.04E-14	[mg.l-1]	O
Continental PEC in seawater (dissolved)	5.28E-14	[mg.l-1]	O
Continental PEC in air (total)	1.98E-14	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.02E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.52E-14	[mg.l-1]	O
Continental PEC in natural soil (total)	1.16E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.16E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.97E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	4.87E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	6.53E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	6.43E-15	[mg.l-1]	O
Moderate PEC in air (total)	5.44E-16	[mg.m-3]	O
Moderate PEC in soil (total)	3.19E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	5.94E-12	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	4.73E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	4.66E-15	[mg.l-1]	O
Arctic PEC in air (total)	1.50E-16	[mg.m-3]	O
Arctic PEC in soil (total)	3.01E-13	[mg.kgwwt-1]	O

Arctic PEC in sediment (total)	4.31E-12	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.77E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.74E-15	[mg.l-1]	O
Tropic PEC in air (total)	2.30E-16	[mg.m-3]	O
Tropic PEC in soil (total)	6.95E-14	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	1.60E-12	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.773	[%]	O
Steady-state mass fraction in regional seawater	0.0763	[%]	O
Steady-state mass fraction in regional air	0.0181	[%]	O
Steady-state mass fraction in regional agricultural soil	1.88	[%]	O
Steady-state mass fraction in regional natural soil	0.242	[%]	O
Steady-state mass fraction in regional industrial soil	0.0895	[%]	O
Steady-state mass fraction in regional freshwater sediment	8.3	[%]	O
Steady-state mass fraction in regional seawater sediment	0.239	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	9.76E-04	[%]	O
Steady-state mass fraction in continental seawater	5.49	[%]	O
Steady-state mass fraction in continental air	0.0203	[%]	O
Steady-state mass fraction in continental agricultural soil	1.06	[%]	O
Steady-state mass fraction in continental natural soil	0.136	[%]	O
Steady-state mass fraction in continental industrial soil	0.0505	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.0105	[%]	O
Steady-state mass fraction in continental seawater sediment	0.861	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	37.3	[%]	O
Steady-state mass fraction in moderate air	6.20E-03	[%]	O
Steady-state mass fraction in moderate soil	0.155	[%]	O
Steady-state mass fraction in moderate sediment	1.17	[%]	O

GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	17.7	[%]	O
Steady-state mass fraction in arctic air	9.35E-04	[%]	O
Steady-state mass fraction in arctic soil	0.0636	[%]	O
Steady-state mass fraction in arctic sediment	0.555	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	23.1	[%]	O
Steady-state mass fraction in tropic air	4.29E-03	[%]	O
Steady-state mass fraction in tropic soil	0.0331	[%]	O
Steady-state mass fraction in tropic sediment	0.723	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	5.29E-03	[kg]	O
Steady-state mass in regional seawater	5.21E-04	[kg]	O
Steady-state mass in regional air	1.24E-04	[kg]	O
Steady-state mass in regional agricultural soil	0.0129	[kg]	O
Steady-state mass in regional natural soil	1.65E-03	[kg]	O
Steady-state mass in regional industrial soil	6.12E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0567	[kg]	O
Steady-state mass in regional seawater sediment	1.63E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	6.67E-06	[kg]	O
Steady-state mass in continental seawater	0.0375	[kg]	O
Steady-state mass in continental air	1.39E-04	[kg]	O
Steady-state mass in continental agricultural soil	7.26E-03	[kg]	O
Steady-state mass in continental natural soil	9.32E-04	[kg]	O
Steady-state mass in continental industrial soil	3.45E-04	[kg]	O
Steady-state mass in continental freshwater sediment	7.15E-05	[kg]	O
Steady-state mass in continental seawater sediment	5.89E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.255	[kg]	O
Steady-state mass in moderate air	4.24E-05	[kg]	O
Steady-state mass in moderate soil	1.06E-03	[kg]	O
Steady-state mass in moderate sediment	7.98E-03	[kg]	O
GLOBAL: ARCTIC			

Steady-state mass in arctic water	0.121	[kg]	O
Steady-state mass in arctic air	6.39E-06	[kg]	O
Steady-state mass in arctic soil	4.35E-04	[kg]	O
Steady-state mass in arctic sediment	3.79E-03	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.158	[kg]	O
Steady-state mass in tropic air	2.93E-05	[kg]	O
Steady-state mass in tropic soil	2.26E-04	[kg]	O
Steady-state mass in tropic sediment	4.94E-03	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	3.46E-09	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	5.52E-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)	5.52E-07	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.27E-03	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	3.45E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	3.45E-08	[mg.l-1]	O
Local PEC in marine sediment during emission episode	7.92E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	6.20E-08	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	6.32E-08	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.20E-07	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.38E-10	[mg.l-1]	O
Local PEC in pore water of grassland	2.63E-10	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.38E-10	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex		S

	V C.11, OECD 209		
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	0.05	[kg.kg-1]	D

sediment			
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	1	[-]	D

inhalation)			
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	??	[mg.l-1]	O

PNEC micro			
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	4.24E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	2.66E-05	[-]	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	1.27E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	7.92E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	3.45E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	1.09E-06	[-]	O
RCR for the regional marine compartment	9.86E-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	1.26E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	1.09E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	9.92E-10	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

22.3 Fluoranthene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	Afa Rütgers 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	DF9C7BF1		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	0	[-]	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	1.97E-03	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	1.45E-03	[ug.m-3]	O
Regional PEC in seawater (total)	1.34E-10	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.26E-09	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	1.28E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	7.58E-13	[mg.m-3]	O
Regional PEC in agricultural soil (total)	7.09E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	4.12E-12	[mg.l-1]	O
Regional PEC in natural soil (total)	7.88E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	7.88E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	5.30E-06	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	5.31E-07	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.38E-14	[mg.l-1]	O
Continental PEC in seawater (total)	6.76E-14	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.20E-14	[mg.l-1]	O
Continental PEC in seawater (dissolved)	6.43E-14	[mg.l-1]	O
Continental PEC in air (total)	3.55E-15	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.33E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.93E-14	[mg.l-1]	O
Continental PEC in natural soil (total)	3.70E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.70E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	5.07E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	2.68E-10	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.40E-14	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.33E-14	[mg.l-1]	O
Moderate PEC in air (total)	2.16E-16	[mg.m-3]	O
Moderate PEC in soil (total)	2.24E-12	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	5.55E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.26E-14	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.20E-14	[mg.l-1]	O
Arctic PEC in air (total)	6.76E-17	[mg.m-3]	O
Arctic PEC in soil (total)	2.23E-12	[mg.kgwwt-1]	O

Arctic PEC in sediment (total)	5.01E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	6.37E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	6.06E-15	[mg.l-1]	O
Tropic PEC in air (total)	2.18E-16	[mg.m-3]	O
Tropic PEC in soil (total)	1.24E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	2.52E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.253	[%]	O
Steady-state mass fraction in regional seawater	0.0261	[%]	O
Steady-state mass fraction in regional air	1.49E-03	[%]	O
Steady-state mass fraction in regional agricultural soil	2.81	[%]	O
Steady-state mass fraction in regional natural soil	0.352	[%]	O
Steady-state mass fraction in regional industrial soil	0.13	[%]	O
Steady-state mass fraction in regional freshwater sediment	10.7	[%]	O
Steady-state mass fraction in regional seawater sediment	0.356	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	2.11E-04	[%]	O
Steady-state mass fraction in continental seawater	2.3	[%]	O
Steady-state mass fraction in continental air	1.21E-03	[%]	O
Steady-state mass fraction in continental agricultural soil	1.16	[%]	O
Steady-state mass fraction in continental natural soil	0.144	[%]	O
Steady-state mass fraction in continental industrial soil	0.0535	[%]	O
Steady-state mass fraction in continental freshwater sediment	8.93E-03	[%]	O
Steady-state mass fraction in continental seawater sediment	1.57	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	26.6	[%]	O
Steady-state mass fraction in moderate air	8.17E-04	[%]	O
Steady-state mass fraction in moderate soil	0.361	[%]	O
Steady-state mass fraction in moderate sediment	3.63	[%]	O

GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	15.7	[%]	O
Steady-state mass fraction in arctic air	1.40E-04	[%]	O
Steady-state mass fraction in arctic soil	0.157	[%]	O
Steady-state mass fraction in arctic sediment	2.14	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	27.7	[%]	O
Steady-state mass fraction in tropic air	1.35E-03	[%]	O
Steady-state mass fraction in tropic soil	0.196	[%]	O
Steady-state mass fraction in tropic sediment	3.77	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	5.20E-03	[kg]	O
Steady-state mass in regional seawater	5.37E-04	[kg]	O
Steady-state mass in regional air	3.06E-05	[kg]	O
Steady-state mass in regional agricultural soil	0.0579	[kg]	O
Steady-state mass in regional natural soil	7.24E-03	[kg]	O
Steady-state mass in regional industrial soil	2.68E-03	[kg]	O
Steady-state mass in regional freshwater sediment	0.22	[kg]	O
Steady-state mass in regional seawater sediment	7.33E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	4.35E-06	[kg]	O
Steady-state mass in continental seawater	0.0473	[kg]	O
Steady-state mass in continental air	2.49E-05	[kg]	O
Steady-state mass in continental agricultural soil	0.0238	[kg]	O
Steady-state mass in continental natural soil	2.97E-03	[kg]	O
Steady-state mass in continental industrial soil	1.10E-03	[kg]	O
Steady-state mass in continental freshwater sediment	1.84E-04	[kg]	O
Steady-state mass in continental seawater sediment	0.0323	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.547	[kg]	O
Steady-state mass in moderate air	1.68E-05	[kg]	O
Steady-state mass in moderate soil	7.43E-03	[kg]	O
Steady-state mass in moderate sediment	0.0747	[kg]	O
GLOBAL: ARCTIC			

Steady-state mass in arctic water	0.322	[kg]	O
Steady-state mass in arctic air	2.87E-06	[kg]	O
Steady-state mass in arctic soil	3.22E-03	[kg]	O
Steady-state mass in arctic sediment	0.0441	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.569	[kg]	O
Steady-state mass in tropic air	2.77E-05	[kg]	O
Steady-state mass in tropic soil	4.03E-03	[kg]	O
Steady-state mass in tropic sediment	0.0776	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	3.88E-10	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	3.05E-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)	3.05E-07	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	2.98E-03	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.91E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.91E-08	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.87E-04	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.89E-08	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.91E-08	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	2.90E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	9.78E-12	[mg.l-1]	O
Local PEC in pore water of grassland	1.48E-11	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	9.78E-12	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V		S

	C.11, OECD 209		
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	0.05	[kg.kg-1]	D

sediment			
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	9.6	[mg.kgdwt-1]	S

PNEC sediment (fresh)			
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	0.0305	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	1.91E-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	1.55E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	9.72E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	1.26E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	1.26E-04	[-]	O
RCR for the regional marine compartment	1.28E-05	[-]	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	2.54E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	2.55E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	5.36E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

22.4 Pyrene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers 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	6B4450B4		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	0	[-]	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	9.19E-04	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	8.08E-04	[ug.m-3]	O
Regional PEC in seawater (total)	7.46E-11	[mg.l-1]	O
Regional PEC in surface water (dissolved)	7.41E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	7.24E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	5.65E-13	[mg.m-3]	O
Regional PEC in agricultural soil (total)	2.38E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	2.29E-12	[mg.l-1]	O
Regional PEC in natural soil (total)	2.60E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	2.60E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	1.88E-06	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	1.80E-07	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	7.93E-15	[mg.l-1]	O
Continental PEC in seawater (total)	3.56E-14	[mg.l-1]	O
Continental PEC in surface water (dissolved)	7.28E-15	[mg.l-1]	O
Continental PEC in seawater (dissolved)	3.45E-14	[mg.l-1]	O
Continental PEC in air (total)	2.60E-15	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.09E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.05E-14	[mg.l-1]	O
Continental PEC in natural soil (total)	1.19E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.19E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.84E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	8.56E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	6.49E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	6.30E-15	[mg.l-1]	O
Moderate PEC in air (total)	1.31E-16	[mg.m-3]	O
Moderate PEC in soil (total)	6.01E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	1.56E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	5.67E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	5.50E-15	[mg.l-1]	O
Arctic PEC in air (total)	4.06E-17	[mg.m-3]	O
Arctic PEC in soil (total)	5.95E-13	[mg.kgwwt-1]	O

Arctic PEC in sediment (total)	1.37E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	2.61E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	2.53E-15	[mg.l-1]	O
Tropic PEC in air (total)	1.12E-16	[mg.m-3]	O
Tropic PEC in soil (total)	2.82E-13	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	6.27E-12	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.347	[%]	O
Steady-state mass fraction in regional seawater	0.0356	[%]	O
Steady-state mass fraction in regional air	2.73E-03	[%]	O
Steady-state mass fraction in regional agricultural soil	2.32	[%]	O
Steady-state mass fraction in regional natural soil	0.285	[%]	O
Steady-state mass fraction in regional industrial soil	0.105	[%]	O
Steady-state mass fraction in regional freshwater sediment	9.28	[%]	O
Steady-state mass fraction in regional seawater sediment	0.296	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	2.98E-04	[%]	O
Steady-state mass fraction in continental seawater	2.97	[%]	O
Steady-state mass fraction in continental air	2.17E-03	[%]	O
Steady-state mass fraction in continental agricultural soil	0.934	[%]	O
Steady-state mass fraction in continental natural soil	0.115	[%]	O
Steady-state mass fraction in continental industrial soil	0.0424	[%]	O
Steady-state mass fraction in continental freshwater sediment	7.97E-03	[%]	O
Steady-state mass fraction in continental seawater sediment	1.23	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	30.2	[%]	O
Steady-state mass fraction in moderate air	1.22E-03	[%]	O
Steady-state mass fraction in moderate soil	0.238	[%]	O
Steady-state mass fraction in moderate sediment	2.51	[%]	O

GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	17.3	[%]	O
Steady-state mass fraction in arctic air	2.06E-04	[%]	O
Steady-state mass fraction in arctic soil	0.103	[%]	O
Steady-state mass fraction in arctic sediment	1.43	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	27.8	[%]	O
Steady-state mass fraction in tropic air	1.70E-03	[%]	O
Steady-state mass fraction in tropic soil	0.109	[%]	O
Steady-state mass fraction in tropic sediment	2.31	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	2.91E-03	[kg]	O
Steady-state mass in regional seawater	2.98E-04	[kg]	O
Steady-state mass in regional air	2.28E-05	[kg]	O
Steady-state mass in regional agricultural soil	0.0194	[kg]	O
Steady-state mass in regional natural soil	2.38E-03	[kg]	O
Steady-state mass in regional industrial soil	8.83E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0777	[kg]	O
Steady-state mass in regional seawater sediment	2.48E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	2.50E-06	[kg]	O
Steady-state mass in continental seawater	0.0249	[kg]	O
Steady-state mass in continental air	1.82E-05	[kg]	O
Steady-state mass in continental agricultural soil	7.82E-03	[kg]	O
Steady-state mass in continental natural soil	9.59E-04	[kg]	O
Steady-state mass in continental industrial soil	3.55E-04	[kg]	O
Steady-state mass in continental freshwater sediment	6.68E-05	[kg]	O
Steady-state mass in continental seawater sediment	0.0103	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.253	[kg]	O
Steady-state mass in moderate air	1.02E-05	[kg]	O
Steady-state mass in moderate soil	1.99E-03	[kg]	O
Steady-state mass in moderate sediment	0.021	[kg]	O
GLOBAL: ARCTIC			

Steady-state mass in arctic water	0.145	[kg]	O
Steady-state mass in arctic air	1.73E-06	[kg]	O
Steady-state mass in arctic soil	8.60E-04	[kg]	O
Steady-state mass in arctic sediment	0.012	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.233	[kg]	O
Steady-state mass in tropic air	1.42E-05	[kg]	O
Steady-state mass in tropic soil	9.16E-04	[kg]	O
Steady-state mass in tropic sediment	0.0193	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	3.65E-10	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.89E-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)	1.89E-07	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.11E-03	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.18E-08	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.18E-08	[mg.l-1]	O
Local PEC in marine sediment during emission episode	6.97E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.04E-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	1.80E-08	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	8.99E-12	[mg.l-1]	O
Local PEC in pore water of grassland	1.52E-11	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	8.99E-12	[mg.l-1]	O
EFFECTS			
INPUT OF EFFECTS DATA			
MICRO-ORGANISMS			
Test system	Respiration inhibition, EU Annex V		S

	C.11, OECD 209		
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	0.05	[kg.kg-1]	D

sediment			
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	140	[mg.kgdwt-1]	S

PNEC sediment (fresh)			
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	8.21E-03	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	5.14E-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	1.99E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local marine sediment compartment	2.49E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the local soil compartment	1.04E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	3.22E-05	[-]	O
RCR for the regional marine compartment	3.15E-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	3.08E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional marine sediment compartment	5.90E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
SOIL			
RCR for the regional soil compartment	2.70E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the regional soil compartment, statistical method	??	[-]	O

22.5 Benz[a]anthracene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers Benzaanthr		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	18438AC6		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	0.026	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.763	[kg.d-1]	S
Daily intake of root crops	0.081	[kg.d-1]	S
Daily intake of meat	0.165	[kg.d-1]	S
Daily intake of dairy products	0.255	[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	0	[-]	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	1.22E-04	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			

INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Type of local STP	With primary settler (9-box)		S
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	5.11E-05	[ug.m-3]	O
Regional PEC in seawater (total)	4.72E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	2.91E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	3.78E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.49E-15	[mg.m-3]	O
Regional PEC in agricultural soil (total)	4.82E-10	[mg.kgdwt-1]	O
Regional PEC in pore water of agricultural soils	4.81E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	6.53E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	6.53E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	6.34E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	8.19E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.04E-16	[mg.l-1]	O
Continental PEC in seawater (total)	3.96E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	5.92E-17	[mg.l-1]	O
Continental PEC in seawater (dissolved)	3.16E-15	[mg.l-1]	O
Continental PEC in air (total)	5.31E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	1.51E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.71E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	2.32E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	2.32E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.29E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	6.86E-11	[mg.kgwwt-1]	O

GLOBAL: MODERATE			
Moderate PEC in water (total)	1.92E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.54E-15	[mg.l-1]	O
Moderate PEC in air (total)	1.55E-18	[mg.m-3]	O
Moderate PEC in soil (total)	6.77E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	3.33E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.89E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.51E-15	[mg.l-1]	O
Arctic PEC in air (total)	5.02E-19	[mg.m-3]	O
Arctic PEC in soil (total)	3.57E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	3.28E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.55E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.24E-15	[mg.l-1]	O
Tropic PEC in air (total)	3.28E-18	[mg.m-3]	O
Tropic PEC in soil (total)	9.66E-13	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	2.69E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0393	[%]	O
Steady-state mass fraction in regional seawater	4.04E-03	[%]	O
Steady-state mass fraction in regional air	1.29E-05	[%]	O
Steady-state mass fraction in regional agricultural soil	0.741	[%]	O
Steady-state mass fraction in regional natural soil	0.128	[%]	O
Steady-state mass fraction in regional industrial soil	0.0474	[%]	O
Steady-state mass fraction in regional freshwater sediment	5.6	[%]	O
Steady-state mass fraction in regional seawater sediment	0.241	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	6.98E-06	[%]	O
Steady-state mass fraction in continental seawater	0.592	[%]	O
Steady-state mass fraction in continental air	7.94E-06	[%]	O
Steady-state mass fraction in continental	0.231	[%]	O

agricultural soil			
Steady-state mass fraction in continental natural soil	0.0399	[%]	O
Steady-state mass fraction in continental industrial soil	0.0148	[%]	O
Steady-state mass fraction in continental freshwater sediment	9.96E-04	[%]	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	9.57	[%]	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	1.84E-04	[kg]	O
Steady-state mass in regional seawater	1.89E-05	[kg]	O
Steady-state mass in regional air	6.03E-08	[kg]	O
Steady-state mass in regional agricultural soil	3.47E-03	[kg]	O
Steady-state mass in regional natural soil	5.99E-04	[kg]	O
Steady-state mass in regional industrial soil	2.22E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0262	[kg]	O
Steady-state mass in regional seawater sediment	1.13E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	3.27E-08	[kg]	O
Steady-state mass in continental seawater	2.77E-03	[kg]	O
Steady-state mass in continental air	3.72E-08	[kg]	O

Steady-state mass in continental agricultural soil	1.08E-03	[kg]	O
Steady-state mass in continental natural soil	1.87E-04	[kg]	O
Steady-state mass in continental industrial soil	6.91E-05	[kg]	O
Steady-state mass in continental freshwater sediment	4.66E-06	[kg]	O
Steady-state mass in continental seawater sediment	8.28E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0749	[kg]	O
Steady-state mass in moderate air	1.21E-07	[kg]	O
Steady-state mass in moderate soil	2.24E-03	[kg]	O
Steady-state mass in moderate sediment	0.0448	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0482	[kg]	O
Steady-state mass in arctic air	2.14E-08	[kg]	O
Steady-state mass in arctic soil	5.16E-04	[kg]	O
Steady-state mass in arctic sediment	0.0289	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.139	[kg]	O
Steady-state mass in tropic air	4.18E-07	[kg]	O
Steady-state mass in tropic soil	3.14E-03	[kg]	O
Steady-state mass in tropic sediment	0.0827	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	3.67E-12	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	8.04E-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)	8.04E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	4.03E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	5.04E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	5.04E-10	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.53E-05	[mg.kgdwt-1]	O

SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.55E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.57E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	2.39E-09	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.57E-13	[mg.l-1]	O
Local PEC in pore water of grassland	2.39E-13	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.57E-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 sediment (fresh)	1.2	[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)	0.601	[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	Yes		S

marine sediment?			
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	1	[-]	D

duration			
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	1	[-]	D

duration			
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	6.70E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	4.20E-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	6.70E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	4.20E-03	[-]	O

Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.97E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	2.43E-06	[-]	O
RCR for the regional marine compartment	3.15E-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	4.85E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	6.26E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	6.10E-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

22.6 Chrysene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers Chrysene		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	2B0DAEA8		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	0.026	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.763	[kg.d-1]	S
Daily intake of root crops	0.081	[kg.d-1]	S
Daily intake of meat	0.165	[kg.d-1]	S
Daily intake of dairy products	0.255	[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	0	[-]	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	1.23E-04	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S

CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	5.89E-05	[ug.m-3]	O
Regional PEC in seawater (total)	5.50E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	3.68E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	4.56E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.15E-15	[mg.m-3]	O
Regional PEC in agricultural soil (total)	4.32E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	6.15E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	7.01E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	7.01E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	6.35E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	7.85E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.82E-16	[mg.l-1]	O
Continental PEC in seawater (total)	6.01E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	1.13E-16	[mg.l-1]	O
Continental PEC in seawater (dissolved)	4.98E-15	[mg.l-1]	O
Continental PEC in air (total)	5.82E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	2.18E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	3.10E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	3.54E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.54E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.96E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	8.57E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	3.62E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	3.00E-15	[mg.l-1]	O
Moderate PEC in air (total)	2.09E-18	[mg.m-3]	O
Moderate PEC in soil (total)	1.27E-12	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	5.16E-11	[mg.kgwwt-1]	O

GLOBAL: ARCTIC			
Arctic PEC in water (total)	3.59E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	2.98E-15	[mg.l-1]	O
Arctic PEC in air (total)	6.88E-19	[mg.m-3]	O
Arctic PEC in soil (total)	6.04E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	5.12E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	3.17E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	2.63E-15	[mg.l-1]	O
Tropic PEC in air (total)	4.74E-18	[mg.m-3]	O
Tropic PEC in soil (total)	2.09E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	4.52E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0256	[%]	O
Steady-state mass fraction in regional seawater	2.65E-03	[%]	O
Steady-state mass fraction in regional air	5.62E-06	[%]	O
Steady-state mass fraction in regional agricultural soil	0.425	[%]	O
Steady-state mass fraction in regional natural soil	0.0776	[%]	O
Steady-state mass fraction in regional industrial soil	0.0287	[%]	O
Steady-state mass fraction in regional freshwater sediment	3.17	[%]	O
Steady-state mass fraction in regional seawater sediment	0.131	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	6.91E-06	[%]	O
Steady-state mass fraction in continental seawater	0.507	[%]	O
Steady-state mass fraction in continental air	4.91E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.188	[%]	O
Steady-state mass fraction in continental natural soil	0.0342	[%]	O
Steady-state mass fraction in continental industrial soil	0.0127	[%]	O
Steady-state mass fraction in continental freshwater sediment	8.56E-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	5.44	[%]	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	0.818	[%]	O
Steady-state mass fraction in tropic sediment	16.8	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	2.12E-04	[kg]	O
Steady-state mass in regional seawater	2.20E-05	[kg]	O
Steady-state mass in regional air	4.66E-08	[kg]	O
Steady-state mass in regional agricultural soil	3.53E-03	[kg]	O
Steady-state mass in regional natural soil	6.44E-04	[kg]	O
Steady-state mass in regional industrial soil	2.38E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0263	[kg]	O
Steady-state mass in regional seawater sediment	1.08E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	5.73E-08	[kg]	O
Steady-state mass in continental seawater	4.20E-03	[kg]	O
Steady-state mass in continental air	4.07E-08	[kg]	O
Steady-state mass in continental agricultural soil	1.56E-03	[kg]	O
Steady-state mass in continental natural soil	2.84E-04	[kg]	O
Steady-state mass in continental industrial soil	1.05E-04	[kg]	O
Steady-state mass in continental freshwater sediment	7.10E-06	[kg]	O
Steady-state mass in continental seawater sediment	0.0104	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.141	[kg]	O

Steady-state mass in moderate air	1.63E-07	[kg]	O
Steady-state mass in moderate soil	4.21E-03	[kg]	O
Steady-state mass in moderate sediment	0.0694	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0914	[kg]	O
Steady-state mass in arctic air	2.92E-08	[kg]	O
Steady-state mass in arctic soil	8.73E-04	[kg]	O
Steady-state mass in arctic sediment	0.0451	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.283	[kg]	O
Steady-state mass in tropic air	6.05E-07	[kg]	O
Steady-state mass in tropic soil	6.78E-03	[kg]	O
Steady-state mass in tropic sediment	0.139	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	4.58E-13	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	9.22E-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)	9.22E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	3.67E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	5.79E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	5.79E-10	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.30E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	9.14E-10	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	9.17E-10	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.04E-09	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.15E-13	[mg.l-1]	O
Local PEC in pore water of grassland	1.30E-13	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.15E-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	0.7	[mg.kgdwt-1]	S

PNEC 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	1	[-]	D

duration			
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	1.32E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	8.27E-05	[-]	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	1.32E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	8.27E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.64E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	5.25E-07	[-]	O
RCR for the regional marine compartment	6.52E-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	1.05E-05	[-]	O

compartment			
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	1.30E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	8.79E-09	[-]	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

22.7 Benzo[a]pyrene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers Benzoapyrene		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	CF6E298B		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	0.026	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.763	[kg.d-1]	S
Daily intake of root crops	0.081	[kg.d-1]	S
Daily intake of meat	0.165	[kg.d-1]	S
Daily intake of dairy products	0.255	[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	0	[-]	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	1.18E-04	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			

Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	4.03E-05	[ug.m-3]	O
Regional PEC in seawater (total)	3.67E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	1.79E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	2.59E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.08E-15	[mg.m-3]	O
Regional PEC in agricultural soil (total)	5.57E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	3.79E-14	[mg.l-1]	O
Regional PEC in natural soil (total)	9.93E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	9.93E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	6.47E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	9.34E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.87E-16	[mg.l-1]	O
Continental PEC in seawater (total)	3.68E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	8.33E-17	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.60E-15	[mg.l-1]	O
Continental PEC in air (total)	7.16E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	3.70E-12	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	2.52E-16	[mg.l-1]	O
Continental PEC in natural soil (total)	6.60E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	6.60E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	3.01E-12	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	9.37E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	2.09E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.48E-15	[mg.l-1]	O
Moderate PEC in air (total)	2.26E-18	[mg.m-3]	O

Moderate PEC in soil (total)	2.08E-12	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	5.32E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	2.07E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.46E-15	[mg.l-1]	O
Arctic PEC in air (total)	7.80E-19	[mg.m-3]	O
Arctic PEC in soil (total)	7.78E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	5.27E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.80E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.27E-15	[mg.l-1]	O
Tropic PEC in air (total)	4.70E-18	[mg.m-3]	O
Tropic PEC in soil (total)	3.62E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	4.57E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0232	[%]	O
Steady-state mass fraction in regional seawater	2.35E-03	[%]	O
Steady-state mass fraction in regional air	6.97E-06	[%]	O
Steady-state mass fraction in regional agricultural soil	0.728	[%]	O
Steady-state mass fraction in regional natural soil	0.146	[%]	O
Steady-state mass fraction in regional industrial soil	0.054	[%]	O
Steady-state mass fraction in regional freshwater sediment	4.29	[%]	O
Steady-state mass fraction in regional seawater sediment	0.206	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	9.45E-06	[%]	O
Steady-state mass fraction in continental seawater	0.413	[%]	O
Steady-state mass fraction in continental air	8.03E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.423	[%]	O
Steady-state mass fraction in continental natural soil	0.0849	[%]	O
Steady-state mass fraction in continental industrial soil	0.0314	[%]	O
Steady-state mass fraction in continental freshwater sediment	1.75E-03	[%]	O
Steady-state mass fraction in continental	1.81	[%]	O

seawater sediment			
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	13.1	[%]	O
Steady-state mass fraction in moderate air	2.82E-05	[%]	O
Steady-state mass fraction in moderate soil	1.1	[%]	O
Steady-state mass fraction in moderate sediment	11.5	[%]	O
GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	8.45	[%]	O
Steady-state mass fraction in arctic air	5.31E-06	[%]	O
Steady-state mass fraction in arctic soil	0.18	[%]	O
Steady-state mass fraction in arctic sediment	7.43	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	25.7	[%]	O
Steady-state mass fraction in tropic air	9.59E-05	[%]	O
Steady-state mass fraction in tropic soil	1.89	[%]	O
Steady-state mass fraction in tropic sediment	22.5	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	1.45E-04	[kg]	O
Steady-state mass in regional seawater	1.47E-05	[kg]	O
Steady-state mass in regional air	4.35E-08	[kg]	O
Steady-state mass in regional agricultural soil	4.54E-03	[kg]	O
Steady-state mass in regional natural soil	9.11E-04	[kg]	O
Steady-state mass in regional industrial soil	3.38E-04	[kg]	O
Steady-state mass in regional freshwater sediment	0.0268	[kg]	O
Steady-state mass in regional seawater sediment	1.29E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	5.90E-08	[kg]	O
Steady-state mass in continental seawater	2.58E-03	[kg]	O
Steady-state mass in continental air	5.01E-08	[kg]	O
Steady-state mass in continental agricultural soil	2.64E-03	[kg]	O
Steady-state mass in continental natural soil	5.30E-04	[kg]	O
Steady-state mass in continental industrial soil	1.96E-04	[kg]	O
Steady-state mass in continental freshwater sediment	1.09E-05	[kg]	O
Steady-state mass in continental seawater sediment	0.0113	[kg]	O
GLOBAL: MODERATE			

Steady-state mass in moderate water	0.0816	[kg]	O
Steady-state mass in moderate air	1.76E-07	[kg]	O
Steady-state mass in moderate soil	6.89E-03	[kg]	O
Steady-state mass in moderate sediment	0.0716	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0528	[kg]	O
Steady-state mass in arctic air	3.32E-08	[kg]	O
Steady-state mass in arctic soil	1.12E-03	[kg]	O
Steady-state mass in arctic sediment	0.0464	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.161	[kg]	O
Steady-state mass in tropic air	5.99E-07	[kg]	O
Steady-state mass in tropic soil	0.0118	[kg]	O
Steady-state mass in tropic sediment	0.141	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	1.21E-13	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	5.73E-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)	5.73E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	4.77E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	3.60E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	3.60E-10	[mg.l-1]	O
Local PEC in marine sediment during emission episode	2.99E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	1.17E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	1.17E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.22E-09	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	7.05E-14	[mg.l-1]	O
Local PEC in pore water of grassland	7.33E-14	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	7.05E-14	[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	0.22	[mg.kgdwt-1]	S

PNEC 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)	1.83	[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	1	[-]	D

duration			
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	2.61E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	1.64E-05	[-]	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	2.61E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	1.64E-04	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	2.21E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	No		S
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	8.14E-07	[-]	O
RCR for the regional marine compartment	1.18E-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	1.63E-05	[-]	O

compartment			
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	2.35E-06	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	1.19E-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

22.8 Benzo[b]fluoranthene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers Benzobflu		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	8EC8647E		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	0.026	[kg.d-1]	S
Daily intake of leaf crops (incl. fruit and cereals)	0.763	[kg.d-1]	S
Daily intake of root crops	0.081	[kg.d-1]	S
Daily intake of meat	0.165	[kg.d-1]	S
Daily intake of dairy products	0.255	[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	0	[-]	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	1.53E-04	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S

Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S
REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	4.97E-05	[ug.m-3]	O
Regional PEC in seawater (total)	4.50E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	2.18E-11	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	3.10E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.07E-14	[mg.m-3]	O
Regional PEC in agricultural soil (total)	2.70E-09	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.84E-13	[mg.l-1]	O
Regional PEC in natural soil (total)	3.74E-09	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	3.74E-09	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	7.87E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	1.12E-07	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.28E-15	[mg.l-1]	O
Continental PEC in seawater (total)	3.01E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	5.61E-16	[mg.l-1]	O
Continental PEC in seawater (dissolved)	2.08E-15	[mg.l-1]	O
Continental PEC in air (total)	1.09E-16	[mg.m-3]	O
Continental PEC in agricultural soil (total)	2.74E-11	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.87E-15	[mg.l-1]	O
Continental PEC in natural soil (total)	3.79E-11	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	3.79E-11	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	2.03E-11	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	7.48E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.08E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	7.43E-16	[mg.l-1]	O
Moderate PEC in air (total)	1.42E-17	[mg.m-3]	O
Moderate PEC in soil (total)	4.94E-12	[mg.kgwwt-1]	O

Moderate PEC in sediment (total)	2.68E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.04E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	7.16E-16	[mg.l-1]	O
Arctic PEC in air (total)	5.12E-18	[mg.m-3]	O
Arctic PEC in soil (total)	2.73E-12	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	2.58E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	7.58E-16	[mg.l-1]	O
Tropic PEC in water (dissolved)	5.22E-16	[mg.l-1]	O
Tropic PEC in air (total)	2.03E-17	[mg.m-3]	O
Tropic PEC in soil (total)	5.32E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	1.88E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0463	[%]	O
Steady-state mass fraction in regional seawater	4.65E-03	[%]	O
Steady-state mass fraction in regional air	1.12E-04	[%]	O
Steady-state mass fraction in regional agricultural soil	5.71	[%]	O
Steady-state mass fraction in regional natural soil	0.887	[%]	O
Steady-state mass fraction in regional industrial soil	0.329	[%]	O
Steady-state mass fraction in regional freshwater sediment	8.43	[%]	O
Steady-state mass fraction in regional seawater sediment	0.398	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	1.04E-04	[%]	O
Steady-state mass fraction in continental seawater	0.546	[%]	O
Steady-state mass fraction in continental air	1.97E-04	[%]	O
Steady-state mass fraction in continental agricultural soil	5.07	[%]	O
Steady-state mass fraction in continental natural soil	0.788	[%]	O
Steady-state mass fraction in continental industrial soil	0.292	[%]	O
Steady-state mass fraction in continental freshwater sediment	0.019	[%]	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	2.86E-04	[%]	O
Steady-state mass fraction in moderate soil	4.23	[%]	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	1.79E-04	[kg]	O
Steady-state mass in regional seawater	1.80E-05	[kg]	O
Steady-state mass in regional air	4.34E-07	[kg]	O
Steady-state mass in regional agricultural soil	0.0221	[kg]	O
Steady-state mass in regional natural soil	3.43E-03	[kg]	O
Steady-state mass in regional industrial soil	1.27E-03	[kg]	O
Steady-state mass in regional freshwater sediment	0.0326	[kg]	O
Steady-state mass in regional seawater sediment	1.54E-03	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	4.03E-07	[kg]	O
Steady-state mass in continental seawater	2.11E-03	[kg]	O
Steady-state mass in continental air	7.63E-07	[kg]	O
Steady-state mass in continental agricultural soil	0.0196	[kg]	O
Steady-state mass in continental natural soil	3.04E-03	[kg]	O
Steady-state mass in continental industrial soil	1.13E-03	[kg]	O
Steady-state mass in continental freshwater sediment	7.34E-05	[kg]	O
Steady-state mass in continental seawater sediment	9.04E-03	[kg]	O
GLOBAL: MODERATE			

Steady-state mass in moderate water	0.0421	[kg]	O
Steady-state mass in moderate air	1.11E-06	[kg]	O
Steady-state mass in moderate soil	0.0164	[kg]	O
Steady-state mass in moderate sediment	0.036	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0265	[kg]	O
Steady-state mass in arctic air	2.17E-07	[kg]	O
Steady-state mass in arctic soil	3.95E-03	[kg]	O
Steady-state mass in arctic sediment	0.0227	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0677	[kg]	O
Steady-state mass in tropic air	2.59E-06	[kg]	O
Steady-state mass in tropic soil	0.0173	[kg]	O
Steady-state mass in tropic sediment	0.0579	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	2.44E-13	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	7.43E-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)	7.43E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	6.18E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	4.66E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	4.66E-10	[mg.l-1]	O
Local PEC in marine sediment during emission episode	3.88E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	4.30E-09	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	4.30E-09	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	4.37E-09	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	2.59E-13	[mg.l-1]	O
Local PEC in pore water of grassland	2.63E-13	[mg.l-1]	O

Local PEC in groundwater under agricultural soil	2.59E-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	0.05	[kg.kg-1]	D

sediment			
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 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)	1.41	[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	??	[-]	O

PNEC oral			
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	4.37E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	2.74E-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	4.37E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	2.74E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.52E-07	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	1.28E-06	[-]	O
RCR for the regional marine compartment	1.82E-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	2.56E-05	[-]	O

compartment			
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	3.63E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	1.08E-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

22.9 Benzo[k]fluoranthene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers 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	1E1AC82D		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	0	[-]	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	6.21E-05	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	2.19E-05	[ug.m-3]	O
Regional PEC in seawater (total)	2.00E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	9.94E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	1.42E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	1.70E-16	[mg.m-3]	O
Regional PEC in agricultural soil (total)	1.06E-10	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	7.55E-15	[mg.l-1]	O
Regional PEC in natural soil (total)	2.09E-10	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	2.09E-10	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	3.43E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	4.89E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	4.40E-17	[mg.l-1]	O
Continental PEC in seawater (total)	2.76E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	2.00E-17	[mg.l-1]	O
Continental PEC in seawater (dissolved)	1.96E-15	[mg.l-1]	O
Continental PEC in air (total)	1.29E-18	[mg.m-3]	O
Continental PEC in agricultural soil (total)	8.01E-13	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	5.72E-17	[mg.l-1]	O
Continental PEC in natural soil (total)	1.58E-12	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	1.58E-12	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	6.88E-13	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	6.73E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.89E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	1.34E-15	[mg.l-1]	O
Moderate PEC in air (total)	5.62E-19	[mg.m-3]	O
Moderate PEC in soil (total)	6.92E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	4.60E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.88E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	1.33E-15	[mg.l-1]	O
Arctic PEC in air (total)	1.96E-19	[mg.m-3]	O

Arctic PEC in soil (total)	2.28E-13	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	4.58E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.72E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	1.22E-15	[mg.l-1]	O
Tropic PEC in air (total)	1.25E-18	[mg.m-3]	O
Tropic PEC in soil (total)	1.35E-12	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	4.18E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0146	[%]	O
Steady-state mass fraction in regional seawater	1.49E-03	[%]	O
Steady-state mass fraction in regional air	1.27E-06	[%]	O
Steady-state mass fraction in regional agricultural soil	0.16	[%]	O
Steady-state mass fraction in regional natural soil	0.0356	[%]	O
Steady-state mass fraction in regional industrial soil	0.0132	[%]	O
Steady-state mass fraction in regional freshwater sediment	2.63	[%]	O
Steady-state mass fraction in regional seawater sediment	0.125	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	2.57E-06	[%]	O
Steady-state mass fraction in continental seawater	0.358	[%]	O
Steady-state mass fraction in continental air	1.67E-06	[%]	O
Steady-state mass fraction in continental agricultural soil	0.106	[%]	O
Steady-state mass fraction in continental natural soil	0.0236	[%]	O
Steady-state mass fraction in continental industrial soil	8.73E-03	[%]	O
Steady-state mass fraction in continental freshwater sediment	4.62E-04	[%]	O
Steady-state mass fraction in continental seawater sediment	1.51	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	13.6	[%]	O
Steady-state mass fraction in moderate air	8.12E-06	[%]	O
Steady-state mass fraction in moderate soil	0.425	[%]	O
Steady-state mass fraction in moderate sediment	11.5	[%]	O

GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	8.87	[%]	O
Steady-state mass fraction in arctic air	1.54E-06	[%]	O
Steady-state mass fraction in arctic soil	0.0612	[%]	O
Steady-state mass fraction in arctic sediment	7.47	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	28.4	[%]	O
Steady-state mass fraction in tropic air	2.96E-05	[%]	O
Steady-state mass fraction in tropic soil	0.813	[%]	O
Steady-state mass fraction in tropic sediment	23.9	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	7.89E-05	[kg]	O
Steady-state mass in regional seawater	8.01E-06	[kg]	O
Steady-state mass in regional air	6.86E-09	[kg]	O
Steady-state mass in regional agricultural soil	8.63E-04	[kg]	O
Steady-state mass in regional natural soil	1.92E-04	[kg]	O
Steady-state mass in regional industrial soil	7.11E-05	[kg]	O
Steady-state mass in regional freshwater sediment	0.0142	[kg]	O
Steady-state mass in regional seawater sediment	6.74E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	1.39E-08	[kg]	O
Steady-state mass in continental seawater	1.93E-03	[kg]	O
Steady-state mass in continental air	9.01E-09	[kg]	O
Steady-state mass in continental agricultural soil	5.72E-04	[kg]	O
Steady-state mass in continental natural soil	1.27E-04	[kg]	O
Steady-state mass in continental industrial soil	4.71E-05	[kg]	O
Steady-state mass in continental freshwater sediment	2.49E-06	[kg]	O
Steady-state mass in continental seawater sediment	8.12E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0735	[kg]	O
Steady-state mass in moderate air	4.38E-08	[kg]	O
Steady-state mass in moderate soil	2.29E-03	[kg]	O
Steady-state mass in moderate sediment	0.0619	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0478	[kg]	O

Steady-state mass in arctic air	8.32E-09	[kg]	O
Steady-state mass in arctic soil	3.30E-04	[kg]	O
Steady-state mass in arctic sediment	0.0403	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.153	[kg]	O
Steady-state mass in tropic air	1.60E-07	[kg]	O
Steady-state mass in tropic soil	4.39E-03	[kg]	O
Steady-state mass in tropic sediment	0.129	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	8.37E-14	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	3.10E-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)	3.10E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	2.46E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.95E-10	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Annual average local PEC in seawater (dissolved)	1.95E-10	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.55E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	2.71E-10	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	2.72E-10	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	3.07E-10	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	1.71E-14	[mg.l-1]	O
Local PEC in pore water of grassland	1.93E-14	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	1.71E-14	[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	1.82E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	1.15E-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	1.82E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	1.15E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	1.00E-08	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	5.85E-07	[-]	O
RCR for the regional marine compartment	8.36E-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	1.17E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	1.67E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	4.44E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional soil compartment, statistical method	??	[-]	O

22.10 Benzo[ghi]perylene

Section/parameter	Actual value	Unit	Stat
STUDY			
STUDY IDENTIFICATION			
Study name	AfA Rütgers Benzoghipery		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	2B1F7ADC		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	0	[-]	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	4.28E-05	[kg.d-1]	S
Total regional emission to surface water	0	[kg.d-1]	S
DISTRIBUTION			
SEWAGE TREATMENT			
REGIONAL			
Indirect emission to agricultural soil	0	[kg.d-1]	S
LOCAL			
[PRODUCTION]			
INPUT AND CONFIGURATION [PRODUCTION]			
INPUT			
Use or bypass STP (local freshwater assessment)	Use STP		S
Use or bypass STP (local marine assessment)	Use STP		S
CONFIGURATION			
Effluent discharge rate of this STP	1.30E+05	[m3.d-1]	S
Calculate dilution from river flow rate	Yes		S
Flow rate of the river	6.81E+05	[m3.d-1]	S

REGIONAL, CONTINENTAL AND GLOBAL DISTRIBUTION			
PECS			
REGIONAL			
Regional PEC in surface water (total)	1.38E-05	[ug.m-3]	O
Regional PEC in seawater (total)	1.25E-12	[mg.l-1]	O
Regional PEC in surface water (dissolved)	5.40E-12	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in seawater (dissolved)	8.15E-13	[mg.l-1]	O
Qualitative assessment might be needed (TGD Part II, 5.6)	No		O
Regional PEC in air (total)	5.24E-17	[mg.m-3]	O
Regional PEC in agricultural soil (total)	3.45E-11	[mg.kgwwt-1]	O
Regional PEC in pore water of agricultural soils	1.92E-15	[mg.l-1]	O
Regional PEC in natural soil (total)	7.15E-11	[mg.kgwwt-1]	O
Regional PEC in industrial soil (total)	7.15E-11	[mg.kgwwt-1]	O
Regional PEC in sediment (total)	2.39E-07	[mg.kgwwt-1]	O
Regional PEC in seawater sediment (total)	3.60E-08	[mg.kgwwt-1]	O
CONTINENTAL			
Continental PEC in surface water (total)	1.09E-17	[mg.l-1]	O
Continental PEC in seawater (total)	1.76E-15	[mg.l-1]	O
Continental PEC in surface water (dissolved)	4.24E-18	[mg.l-1]	O
Continental PEC in seawater (dissolved)	1.14E-15	[mg.l-1]	O
Continental PEC in air (total)	3.35E-19	[mg.m-3]	O
Continental PEC in agricultural soil (total)	2.21E-13	[mg.kgwwt-1]	O
Continental PEC in pore water of agricultural soils	1.23E-17	[mg.l-1]	O
Continental PEC in natural soil (total)	4.57E-13	[mg.kgwwt-1]	O
Continental PEC in industrial soil (total)	4.57E-13	[mg.kgwwt-1]	O
Continental PEC in sediment (total)	1.88E-13	[mg.kgwwt-1]	O
Continental PEC in seawater sediment (total)	5.05E-11	[mg.kgwwt-1]	O
GLOBAL: MODERATE			
Moderate PEC in water (total)	1.21E-15	[mg.l-1]	O
Moderate PEC in water (dissolved)	7.88E-16	[mg.l-1]	O
Moderate PEC in air (total)	1.65E-19	[mg.m-3]	O
Moderate PEC in soil (total)	2.25E-13	[mg.kgwwt-1]	O
Moderate PEC in sediment (total)	3.48E-11	[mg.kgwwt-1]	O
GLOBAL: ARCTIC			
Arctic PEC in water (total)	1.21E-15	[mg.l-1]	O
Arctic PEC in water (dissolved)	7.84E-16	[mg.l-1]	O
Arctic PEC in air (total)	5.56E-20	[mg.m-3]	O

Arctic PEC in soil (total)	6.79E-14	[mg.kgwwt-1]	O
Arctic PEC in sediment (total)	3.47E-11	[mg.kgwwt-1]	O
GLOBAL: TROPIC			
Tropic PEC in water (total)	1.11E-15	[mg.l-1]	O
Tropic PEC in water (dissolved)	7.19E-16	[mg.l-1]	O
Tropic PEC in air (total)	3.84E-19	[mg.m-3]	O
Tropic PEC in soil (total)	4.68E-13	[mg.kgwwt-1]	O
Tropic PEC in sediment (total)	3.17E-11	[mg.kgwwt-1]	O
STEADY-STATE FRACTIONS			
REGIONAL			
Steady-state mass fraction in regional freshwater	0.0134	[%]	O
Steady-state mass fraction in regional seawater	1.35E-03	[%]	O
Steady-state mass fraction in regional air	5.68E-07	[%]	O
Steady-state mass fraction in regional agricultural soil	0.0757	[%]	O
Steady-state mass fraction in regional natural soil	0.0176	[%]	O
Steady-state mass fraction in regional industrial soil	6.53E-03	[%]	O
Steady-state mass fraction in regional freshwater sediment	2.66	[%]	O
Steady-state mass fraction in regional seawater sediment	0.133	[%]	O
CONTINENTAL			
Steady-state mass fraction in continental freshwater	9.18E-07	[%]	O
Steady-state mass fraction in continental seawater	0.33	[%]	O
Steady-state mass fraction in continental air	6.30E-07	[%]	O
Steady-state mass fraction in continental agricultural soil	0.0424	[%]	O
Steady-state mass fraction in continental natural soil	9.87E-03	[%]	O
Steady-state mass fraction in continental industrial soil	3.65E-03	[%]	O
Steady-state mass fraction in continental freshwater sediment	1.83E-04	[%]	O
Steady-state mass fraction in continental seawater sediment	1.64	[%]	O
GLOBAL: MODERATE			
Steady-state mass fraction in moderate water	12.7	[%]	O
Steady-state mass fraction in moderate air	3.45E-06	[%]	O
Steady-state mass fraction in moderate soil	0.2	[%]	O
Steady-state mass fraction in moderate sediment	12.6	[%]	O

GLOBAL: ARCTIC			
Steady-state mass fraction in arctic water	8.25	[%]	O
Steady-state mass fraction in arctic air	6.35E-07	[%]	O
Steady-state mass fraction in arctic soil	0.0263	[%]	O
Steady-state mass fraction in arctic sediment	8.19	[%]	O
GLOBAL: TROPIC			
Steady-state mass fraction in tropic water	26.5	[%]	O
Steady-state mass fraction in tropic air	1.31E-05	[%]	O
Steady-state mass fraction in tropic soil	0.409	[%]	O
Steady-state mass fraction in tropic sediment	26.2	[%]	O
STEADY-STATE MASSES			
REGIONAL			
Steady-state mass in regional freshwater	4.98E-05	[kg]	O
Steady-state mass in regional seawater	5.01E-06	[kg]	O
Steady-state mass in regional air	2.12E-09	[kg]	O
Steady-state mass in regional agricultural soil	2.82E-04	[kg]	O
Steady-state mass in regional natural soil	6.56E-05	[kg]	O
Steady-state mass in regional industrial soil	2.43E-05	[kg]	O
Steady-state mass in regional freshwater sediment	9.91E-03	[kg]	O
Steady-state mass in regional seawater sediment	4.97E-04	[kg]	O
CONTINENTAL			
Steady-state mass in continental freshwater	3.42E-09	[kg]	O
Steady-state mass in continental seawater	1.23E-03	[kg]	O
Steady-state mass in continental air	2.35E-09	[kg]	O
Steady-state mass in continental agricultural soil	1.58E-04	[kg]	O
Steady-state mass in continental natural soil	3.67E-05	[kg]	O
Steady-state mass in continental industrial soil	1.36E-05	[kg]	O
Steady-state mass in continental freshwater sediment	6.81E-07	[kg]	O
Steady-state mass in continental seawater sediment	6.10E-03	[kg]	O
GLOBAL: MODERATE			
Steady-state mass in moderate water	0.0472	[kg]	O
Steady-state mass in moderate air	1.28E-08	[kg]	O
Steady-state mass in moderate soil	7.45E-04	[kg]	O
Steady-state mass in moderate sediment	0.0468	[kg]	O
GLOBAL: ARCTIC			
Steady-state mass in arctic water	0.0307	[kg]	O

Steady-state mass in arctic air	2.37E-09	[kg]	O
Steady-state mass in arctic soil	9.81E-05	[kg]	O
Steady-state mass in arctic sediment	0.0305	[kg]	O
GLOBAL: TROPIC			
Steady-state mass in tropic water	0.0987	[kg]	O
Steady-state mass in tropic air	4.89E-08	[kg]	O
Steady-state mass in tropic soil	1.52E-03	[kg]	O
Steady-state mass in tropic sediment	0.0977	[kg]	O
LOCAL PECS [PRODUCTION]			
AIR			
Annual average local PEC in air (total)	2.82E-14	[mg.m-3]	O
WATER, SEDIMENT			
Local PEC in surface water during emission episode (dissolved)	1.81E-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)	1.81E-09	[mg.l-1]	O
Local PEC in fresh-water sediment during emission episode	1.85E-04	[mg.kgdwt-1]	O
Local PEC in seawater during emission episode (dissolved)	1.14E-10	[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-10	[mg.l-1]	O
Local PEC in marine sediment during emission episode	1.16E-05	[mg.kgdwt-1]	O
SOIL, GROUNDWATER			
Local PEC in agric. soil (total) averaged over 30 days	9.30E-11	[mg.kgdwt-1]	O
Local PEC in agric. soil (total) averaged over 180 days	9.33E-11	[mg.kgdwt-1]	O
Local PEC in grassland (total) averaged over 180 days	1.06E-10	[mg.kgdwt-1]	O
Local PEC in pore water of agricultural soil	4.57E-15	[mg.l-1]	O
Local PEC in pore water of grassland	5.17E-15	[mg.l-1]	O
Local PEC in groundwater under agricultural soil	4.57E-15	[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	2.21E-04	[-]	O
Intermittent release	No		D
RCR for the local marine compartment	1.39E-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	2.21E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local marine sediment compartment	1.39E-03	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the local soil compartment	5.56E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the local soil compartment, statistical method	??	[-]	O
STP			
RCR for the sewage treatment plant	??	[-]	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	6.59E-07	[-]	O
RCR for the regional marine compartment	9.93E-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	1.32E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional marine sediment compartment	1.98E-05	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
SOIL			
RCR for the regional soil compartment	2.34E-09	[-]	O
Extra factor 10 applied to PEC/PNEC	Yes		O
RCR for the regional soil compartment, statistical method	??	[-]	O

23 ANNEX XII – BIOMONITORING CAMPAIGN

Methods

A biomonitoring campaign was performed recently. Samples were taken from different groups of workers in September 2018. All raw data are presented below.

Samples were taken at the end of shift or in case of maintenance workers after finishing a task with possible exposure (no further information on the tasks performed available). Importantly, all samples were taken contamination free. This means that specimen collection was performed after taking off the work clothes and washing hands or showering at the end of the activities involved. Collection was carried out directly in the urine cup. Most participating workers provided more than 1 sample.

Analysis of samples was performed by "Medizinisches Labor Bremen" (Dr. H.-W.-Hoppe/Dr. Heitland). The respective laboratory is certified for assessment of 1-OHP in urine according to German External Quality Assessment Scheme from the 60^{th} ring trial 2017 for toxicological analyses in biological material (LOQ in urine: < 0,1 µg/L).

Results

For details see separate file „Confidential information on biomonitoring results-raw data.pdf" attached to IUCLID section 13.

24 ANNEX XIII – ART PROTOCOL

ART REPORT – CTPht - RÜTGERS Germany – Fire brigade worker –barge loading (PROC 8b) far field – 13-Feb-19	
PROC 8b - Transfer of substance (charging/discharging) from/to vessels/large containers at dedicated facilities	
Chemical details	
Chemical	BaP
CAS No.	50-32-8
Scenario details	
Number of activities	1
Total duration (mins)	480
Nonexposure period (mins)	477
Metadata	
ART version	1.5
Date created	29-Nov-17
Date last edited	13-Feb-19
Details for Activity Transfer dedicated facilities - barge loading	
Duration (mins):	3
Emission sources:	Near field
	Far field ✓
Far-field exposure	
Operational Conditions	
Substance emission potential	
Substance product type	Liquids
Process temperature	[redacted]
Vapour pressure	0.98 Pa
Liquid weight fraction	0.00873
Viscosity	Medium
Activity emission potential	
Activity class	Falling liquids
Situation	Transfer of liquid product with flow of > 1000 l/minute
Containment level	Open process
Loading type	Splash loading, where the liquid dispenser remains at the top of the reservoir and the liquid splashes freely
Surface contamination	
Process fully enclosed?	No
Effective housekeeping practices in place?	Yes
Dispersion	
Work area	Outdoors
Source located close to buildings?	No

Worker distance	> 4 m
Risk Management Measures	
Localised controls	
Primary	Vapour recovery systems (80.00 % reduction)
Secondary	No localized controls (0.00 % reduction)
Segregation	No segregation (0.00 % reduction)
Personal enclosure	No personal enclosure (0.00 % reduction)
Predicted exposure levels	
ART predicts air concentrations in a worker's personal breathing zone outside of any Respiratory Protection Equipment (RPE). The use of RPE must be considered separately.	
Mechanistic model results	
The predicted 90th percentile full-shift exposure is 0.00000019 mg/m³.	
The inter-quartile confidence interval is 0.000000075 mg/m³ to 0.00000056 mg/m³.	