

Annex XV dossier

**PROPOSAL FOR IDENTIFICATION OF A SUBSTANCE AS A
CMR CAT 1 OR 2, PBT, vPvB OR A SUBSTANCE OF AN
EQUIVALENT LEVEL OF CONCERN**

Substance Name: Anthracene oil, anthracene-low

EC Number: 292-604-8

CAS Number: 90640-82-7

Submitted by: Germany

Version: August 2009

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Substance Name: Anthracene oil, anthracene low

EC Number: 292-604-8

CAS number: 90640-82-7

- *It is proposed to identify the substance as a PBT according to Article 57 (d).*
- *It is proposed to identify the substance as a vPvB according to Article 57 (e).*

Summary of how the substance meets the CMR (Cat 1 or 2), PBT or vPvB criteria, or is considered to be a substance of an equivalent level of concern

Anthracene oil, anthracene low is a UVCB substance consisting of different constituents, among them various PAH. One relevant constituent is anthracene which is present in anthracene oil, anthracene low in the range of 1-6%. Anthracene has been placed on the Candidate List due to the identification as a PBT-substance. Moreover, anthracene oil, anthracene low consists of further PAH such as phenanthrene, fluoranthene, and pyrene which fulfil the PBT and vPvB criteria, too.

Hence, anthracene oil fulfils the PBT, and the vPvB, criteria according to article 57 d) and e) of the REACH regulation.

Registration number(s) of the substance or of substances containing the substance:

JUSTIFICATION

1 IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

1.1 Name and other identifiers of the substance

Chemical Name: Anthracene oil, anthracene-low

EC Number: 292-604-8

CAS Number: 90640-82-7

IUPAC Name:

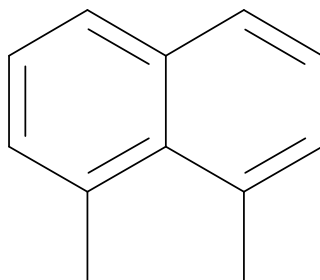
1.2 Composition of the substance

Anthracene oil, anthracene-low (CAS Number 90640-82-7)

The anthracene oil, anthracene low derivatives are complex and have variable compositions.

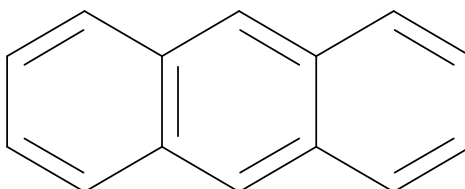
According to the EC inventory the oil remaining after the removal, by a crystallization process, of an anthracene-rich solid (anthracene paste) from anthracene oil. It is composed primarily of two, three and four membered aromatic compounds. The data provided by industry in the IUCLID files show, that the composition of anthracene-oil is as follows:

Chemical Name:	Acenaphthene
EC Number:	201-469-6
CAS Number:	83-32-9
IUPAC Name:	1,2-dihydroacenaphthylene
Molecular Formula:	C ₁₂ H ₁₀
Structural Formula:	



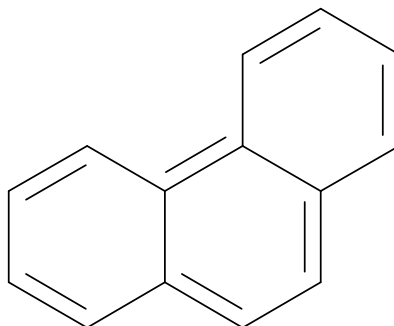
Molecular Weight:	154.21
Typical concentration (% w/w):	
Concentration range (% w/w):	1 – 10

Chemical Name: Anthracene
EC Number: 204-371-1
CAS Number: 120-12-7
IUPAC Name: Anthracene
Molecular Formula: C₁₄H₁₀
Structural Formula:



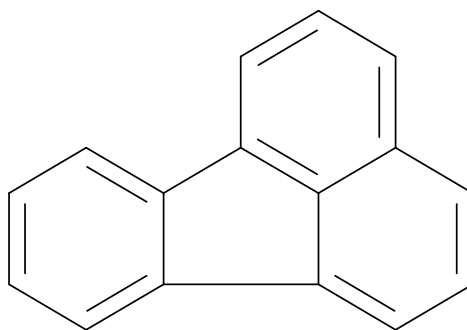
Molecular Weight: 178.23
Typical concentration (% w/w):
Concentration range (% w/w): 1 - 6

Chemical Name: Phenanthrene
EC Number: 201-581-5
CAS Number: 85-01-8
IUPAC Name: Phenanthrene
Molecular Formula: C₁₄H₁₀
Structural Formula:



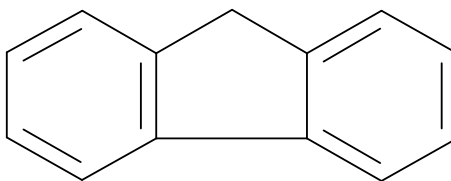
Molecular Weight: 178.23
Typical concentration (% w/w):
Concentration range (% w/w): 10 – 30

Chemical Name: Fluoranthene
EC Number: 205-912-4
CAS Number: 206-44-0
IUPAC Name: Fluoranthene
Molecular Formula: C₁₆H₁₀
Structural Formula:



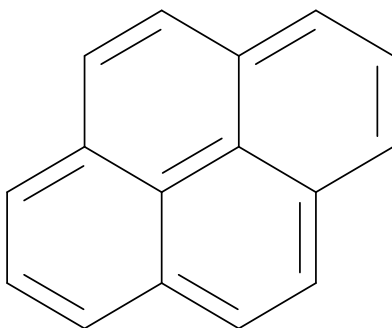
Molecular Weight: 202.26
Typical concentration (% w/w):
Concentration range (% w/w): 5 - 15

Chemical Name: Fluorene
EC Number: 201-695-5
CAS Number: 86-73-7
IUPAC Name: 9H-fluorene
Molecular Formula: C₁₃H₁₀
Structural Formula:



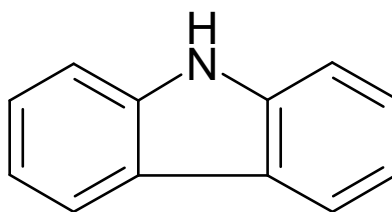
Molecular Weight: 166.22
Typical concentration (% w/w):
Concentration range (% w/w): 4 – 10

Chemical Name: Pyrene
EC Number: 204-927-3
CAS Number: 129-00-0
IUPAC Name: Pyrene
Molecular Formula: C₁₆H₁₀
Structural Formula:



Molecular Weight: 202.26
Typical concentration (% w/w):
Concentration range (% w/w): 2 – 8

Chemical Name: Carbazole
EC Number: 201-696-0
CAS Number: 86-74-8
IUPAC Name: 9H-carbazole
Molecular Formula: C₁₂H₉N
Structural Formula:



Molecular Weight: 167.21
Typical concentration (% w/w):
Concentration range (% w/w): 1 – 3

1.3 Physico-chemical properties

Table 1: Summary of the physico-chemical properties

REACH ref Annex, §	Property	IUCLID section	Value	[enter comment/reference or delete column]
VII, 7.1	Physical state at 20°C and 101.3 kPa	3.1	liquid	IUCLID data file
VII, 7.2	Melting/freezing point	3.2	20-70 °C	IUCLID data file; Depending on the concentration of the different substances
VII, 7.3	Boiling point	3.3	230-400 °C	IUCLID data file; Depending on the concentration of the different substances
VII, 7.5	Vapour pressure	3.6	≤ 200 Pa	IUCLID data file
VII, 7.7	Water solubility	3.8	< 100 mg/l	IUCLID data file; Depending on the concentration of the different substances
VII, 7.8	Partition coefficient n-octanol/water (log value)	3.7 partition coefficient	3.84 – 5.20	IUCLID data file: Depending on the concentration of the different substances

2 MANUFACTURE AND USES

Not relevant for this type of dossier.

3 CLASSIFICATION AND LABELLING**3.1 Classification in Annex VI of Regulation (EC) No 1272/2008**

Anthracene oil, anthracene low has index number 648-104-00 in Annex VI, part 3, Tables 3.1 and 3.2 of Regulation (EC) No 1272/2008.

Its classification according to part 3 of Annex VI, Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Regulation (EC) No 1272/2008) and of its constituents addressed in this dossier is provided in Table 2.

Table 2: Classification and labelling of anthracene oil, anthracene low according to Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008.

Name	Cas-No	Index-No	Classification	Labelling
Anthracen oil, anthracene-low [#]	90640-82-7	648-104-00-0	Carc. Cat. 2; R45 *	T; R45; S 53 – 45

[#]The classification and label shown for this substance applies to the dangerous property indicated by the risk phrases in combination with the category of danger shown. Manufacturers, importers and downstream users of this substance shall be obliged to carry out an investigation to make themselves aware of the relevant and accessible data which exists for all other properties to classify and label the substance. The final label shall follow the requirements of section 7 of Annex VI to Directive 67/548/EEC; * The classification as a carcinogen need not apply if it can be shown that the substance contains less than 0,005 % w/w benzo[a]-pyrene (EINECS No 200-028-5)

The harmonised classification and labelling of anthracene oil, anthracene paste as hazardous substances according to Regulation (EC) No 1272/2008 (Annex VI, part 3, Table 3.1) is provided in Table 3.

Table 3: Classification and labelling of anthracene oil, anthracene low according to Annex VI, part 3, Table 3.1 of Regulation (EC) No 1272/2008.

Name	Cas-No	Index-No	Classification	Labelling
Anthracene oil, anthracene low [#] ,	90640-82-7	648-104-00-0	Carc. Cat. 1B* H350	GHS08 Dgr H350

[#] The classification and labelling shown for this substance applies to the hazardous property(ies) indicated by the hazard statement(s) in combination with the hazard class(es) and category(ies) shown. The requirements of Article 4 (Regulation (EC) No. 1272/2008) for manufacturers, importers or downstream users of this substance apply to all other hazard classes and categories.; *The classification as a carcinogen need not apply if it can be shown that the substance contains less than 0,005 % w/w benzo[a]-pyrene (EINECS No 200-028-5).

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation

4.1.1 Stability

4.1.1.1 Phototransformation

Photolysis in the troposphere results in the formation of reactive hydroxyl (OH) and nitrate (NO₃) radicals and ozone (O₃), which react as oxidizing agent with organic compounds, like PAHs. These radical and ozone reactions comprise mainly the degradation of gas-phase PAH (Calvert *et al.*, 2002). The atmospheric behaviour of the main constituent of anthracene oil, anthracene low¹ is shown below in Table 4.

Table 4: Phototransformation of the relevant constituents of anthracene oil, anthracene low. Data are taken from the Annex XV transitional report for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009)

PAH (number of rings)	Representative lifetime in air with respect to reaction with			
	OH		NO ₃	O ₃
	Summer	Winter		
Phenanthrene (2)	9.0 h	1.9 d	-	-
Fluoranthene (4)	5.6 h	1.2 d	340 d	-
9H-Fluorene (3)	1.8 h	9 d	-	-
Pyrene (4)	5.6 h	1.2 d	120 d	-
Acenaphthene (3)	3.5 h	18 h	4.8 h	> 30 d
Carbazole (2) ^{a)}	9.63 h	-	-	-

a) especially calculated for this dossier with AOPwin v1.91.

For all of these substances the transformation rate in particle phase is expected to be lower. Particle phase transformation is, however, not assumed to be of relevance for the overall atmospheric lifetime, because e.g. only up to 3% of atmospheric anthracene, anthracene low has been observed to appear in particle phase (European Chemical Agency, 2008d).

Environmentally relevant exposure occurs in the whole water column and, in the case of anthracene oil, anthracene low especially in sediment and soil. Photodegradation of anthracene oil, anthracene low can be expected to be a relevant removal pathway in the environment only in very shallow clear waters and in the first few centimetres layer of the water column. Therefore aquatic photodegradation is not considered to have relevant impact on the overall persistency of anthracene oil, anthracene low in the environment.

¹ Please note that data relevant for the constituent anthracene are not shown in this dossier, since anthracene has already been identified as a PBT substance (European Chemicals Agency, 2008).

4.1.1.2 Hydrolysis

Hydrolysis as a way of abiotic degradation can be considered as not relevant for the main substances constituents because of their chemical structures. E.g. the constituent anthracene is stable against hydrolysis, photochemical transformation in water and sediments. This has been observed in laboratory and in “in situ” experiments. Half-lives for primary photodegradation in water have been reported in the range of 20 minutes to 125 hours depending on the experimental conditions used. The highest value corresponds to photolysis in winter conditions. Anthraquinone has been identified as the main abiotic degradation product of anthracene (European Chemical Agency, 2008d). Because of the similar chemical structure (consisting of aromatic rings) similar assumptions for hydrolytic behaviour of the other anthracene oil, anthracene low constituents can be made.

4.1.2 Biodegradation

4.1.2.1 Biodegradation estimation

4.1.2.2 Screening tests

The PAH listed in the table below were allocated on the basis of model calculations (Mackay *et al.*, 1992). These half-lives were applied in the Annex XV transitional report for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009)

Table 5: Ranking of PAH in different half-life classes according to (The Netherlands - Bureau REACH, 2009)

Substance	Water		Soil		Sediment	
	class	Half-life [d]	class	Half-life [d]	class	Half-life [d]
Acenaphthene	3	5 – 13	5	42 – 125	6	125 – 420
Fluorene	4	13 – 42	6	125 – 420	7	420 – 1250
Phenanthrene	4	13 – 42	6	125 – 420	7	420 – 1250
Fluoranthene	4	13 – 42	7	420 – 1250	8	>1250
Pyrene	5	42 – 125	7	420 – 1250	8	>1250

In a 28 day ready biodegradability test (MITI I, OECD 301C) using 100 mg l⁻¹ PAH, respectively, and 30 mg l⁻¹ sludge readily biodegradation was detected for phenanthrene. For fluorene, carbazole and acenaphthene no biodegradation was measured (Table 6). According to the MITI test, which is suitable for substances with low water solubility, these PAH are not readily biodegradable (MITI-List, 2002).

Table 6: Biodegradation of several PAH according to the test method MITI I (OECD TG 301C).

Compound	BOD	Judgement
Phenanthrene	54,0	Ready biodegradable
Fluorene	0 %	Not-biodegradable
Carbazole	0 %	Not-biodegradable
Acenaphthene	0%	Not-biodegradable

Coover and Sims tested the persistence of PAHs in an unacclimated agricultural sandy loam soil in dependence of the temperature (Coover and Sims, 1987). Due to the method used for extraction and analysis, it remains unclear to which extent evaporation, adsorption and biodegradation may have contributed to the elimination process. The soil was spiked with a standard solution of 16 PAHs and incubated for 240 days. At 10°C 36% of phenanthrene, 94% of fluoranthene and 93% of pyrene were remaining. With increasing temperature the degradation increased. 19% (2%) of phenanthrene, 71% (15%) of fluoranthene and 89% (43%) of pyrene were remaining at 20°C (30°C).

4.1.2.3 Simulation tests

Biodegradation in soil

Biodegradation rates of several PAH in soil depend on several factors like soil type, pH, moisture content, oxygen and nutrient contents and soil microbial population. In addition, vegetation has been observed to enhance microbial biodegradation in the rhizosphere. Some of these factors may also explain why the half-lives observed under laboratory conditions are much shorter than those obtained from long-term field-based experiments (The Netherlands - Bureau REACH, 2009). The results of Wild et al. (1991) and Wild and Jones (1993) demonstrate the difference of tests conducted for several PAHs in field conditions compared to laboratory tests. Wild et al. (1991) observed an elimination half-life of 5.7 years for phenanthrene, 7.8 years for fluoranthene, and 8.5 years for pyrene. In this field experiment soils were enriched with PAH-contaminated sludge (Wild *et al.*, 1991).

In another study Wild and Jones (1993) derived different half-lives in a microcosm study with four soil types (Wild and Jones, 1993). The elimination half-lives for the PAH tested are as follows: phenanthrene 83 – 193 days; fluoranthene 110 – 184 days; and pyrene 127 - 320 days. It has to be noted that the latter results are derived from a greenhouse study and should therefore not be used for the P-assessment. Various studies on PAH-contaminated soils have shown that the number of PAH-degrading microorganisms and the degrading capacity are much higher in PAH-contaminated soils than in pristine soils indicating that adaptation has occurred (The Netherlands - Bureau REACH, 2009).

Grosser et al. studied the mineralization of ¹⁴C-labeled pyrene and carbazole in three different soils (Grosser *et al.*, 1991). The mineralization was measured by application of serum bottle radiorespirometry. The incubation was set up for 184 days, but after 60 days the curves had become asymptotic. The mineralization of pyrene was measured between 10 and 48% and for carbazole between undetectable and 46% within the test duration.

The fate of several PAHs in two different soils were tested by Park et al. (Park *et al.*, 1990). The half-life of phenanthrene was calculated in the range of 27 and 53 days (second soil: 13 – 18 days), a half life of fluoranthene between 173 and 630 days (second soil: 277 – 578 days) and a half life of pyrene between 131 and 408 days (second soil: 193 – 408 days).

Table 7: Half-lives of relevant compounds present in anthracene oil

Substance	Result	Reference
Phenanthrene	DisDT ₅₀ = 5.7 years (field study)	(Wild <i>et al.</i> , 1991)
	DisDT ₅₀ = 83 – 193 d (microcosm study)	(Wild and Jones, 1993)
	Elimination half- life in two different soils: DisDT ₅₀ = 27 – 53 d DisDT ₅₀ = 13 – 18 d	(Park <i>et al.</i> , 1990)
Fluoranthene	DisDT ₅₀ = 7.8 years (field study)	(Wild <i>et al.</i> , 1991)
	DisDT ₅₀ = 110 – 184 d (microcosm study)	(Wild and Jones, 1993)
	Elimination half- life in two different soils: DisDT ₅₀ = 173 – 630 d DisDT ₅₀ = 277 – 578 d	(Park <i>et al.</i> , 1990)
Pyrene	Degradation half-life: DegDT ₅₀ > 184 d (10 – 48 % mineralization in 184 d)	(Grosser <i>et al.</i> , 1991)
	DisDT ₅₀ = 8.5 years (field study)	(Wild <i>et al.</i> , 1991)
	DisDT ₅₀ = 127 - 320 d	(Wild and Jones, 1993)
	Elimination half- life in two different soils: DisDT ₅₀ = 131 – 408 d DisDT ₅₀ = 193 – 408 d	(Park <i>et al.</i> , 1990)
Carbazole	Degradation half-life: DegDT ₅₀ > 184 d (undetectable – 46 % mineralization in 184 d)	(Grosser <i>et al.</i> , 1991)

4.1.3 Summary and discussion of persistence

Anthracene which is one relevant constituent of anthracene oil, anthracene low has been placed on the Candidate List due to the identification as a PBT-substance (European Chemicals Agency, 2008).

Moreover, anthracene oil, anthracene low consists of further hardly degradable PAHs. The model calculations by Mackay *et al.* (1992) indicate that acenaphthene, fluorene, phenanthrene, fluoranthene, and pyrene show half-times in sediment > 180 days.

Screening studies (OECD TG 301C) show, that acenaphthene, fluorene and carbazole – constituents present in anthracene oil, anthracene low - are not readily biodegradable (MITI-List, 2002).

Further studies show relatively long dissipation times for fluoranthene (DisDT₅₀ > 173 d), pyrene (DisDT₅₀ > 131 d), and carbazole (DegDT₅₀ > 184 d) (Park *et al.*, 1990; Grosser *et al.*, 1991).

Additionally in a field study half lives of 5.7 years for phenanthrene, 7.8 years for fluoranthene, and 8.5 years for pyrene, have been measured in soil (Wild *et al.*, 1991).

Hence, several constituents of anthracene oil fulfil the P, and the vP criteria according to article 57 d) and e) of the REACH regulation.

4.2 Environmental distribution

4.2.1 Adsorption/desorption

The organic carbon partitioning coefficient $\log K_{OC}$ was calculated for the main constituents using the equation $\log K_{OC} = 0.81 * \log K_{OW} + 0.10$ (European Chemicals Agency, 2008). The results are shown below in Table 8.

Table 8: $\log K_{OW}$ and $\log K_{OC}$ data of the relevant constituents of anthracene oil, anthracene low.

Substance	CAS-No.	$\log K_{OW}$ ^{a)}	$\log K_{OC}$	K_{OC} (l/kg) ^{b)}
Phenanthrene	85-01-8	4.57	3.80	6309
Anthracene	120-12-7	4.68	3.89	7762
Fluoranthene	206-44-0	5.20	4.31	20417
Fluorene	86-73-7	4.22	3.52	3311
Pyrene	129-00-0	4.98	4.13	13489
Acenaphthene	83-32-9	4.00	3.34	2187
Carbazole	86-74-8	3.84	3.21	1621

a) Values taken from Annex XV Transitional Dossier – CTPht (The Netherlands - Bureau REACH, 2009) b) calculation of K_{OC} according to Guidance document R.7a

It can be concluded that anthracene oil, anthracene low has a high potential to adsorb to organic matter and that it is not or only little mobile in soil and sediment.

4.2.2 Volatilisation

For the substance anthracene oil, anthracene low no measured data are available at the moment. According to the constituent's Henry' Law constants anthracene oil, anthracene low is appreciated to be moderately volatile. The calculated values are shown in

Table 9 using the equation for Henry's law constant documented in Guidance Document R.16 (European Chemicals Agency, 2008b).

4.2.3 Distribution modelling

For the main constituents of anthracene oil the behaviour in the wastewater treatment plant was calculated under the assumption that no biodegradation occurs ($k=0/h$). The results are shown in

Table 9.

Table 9: Henry constants and volatilisation of main constituents in municipal waste water treatment plants.

Substance	Henry-constant ^a (Pa*m ³ /mol)	Distribution of PAH in STP ^b			
		% to air	% to water	% to sludge	% degraded
Phenanthrene	4.76	4.4	53.5	42.1	0.0
Anthracene	3.56	3.1	50.0	46.9	0.0
Fluoranthene	0.14	0.6	31.7	67.7	0.0
Fluorene	7.57	8.5	63.6	27.9	0.0
Pyrene	1.62	1.1	39.3	59.6	0.0
Acenaphthene	13.01	14.5	65.2	20.3	0.0
Carbazole	0.01	0.0	83.3	16.7	0.0

^a calculation of Henry's law coefficient according to Guidance document R.16 (European Chemicals Agency, 2008); ^b values for distribution in STP calculated with SimpleTreat 3.0 (debugged version, 7 Feb 97)

Due to the partitioning to solids, low concentrations of PAHs in aqueous solutions are expected. The share of anthracene oil, anthracene low constituents volatilised depends on the composition of the oil. Nevertheless volatilisation is not considered as a relevant route of distribution for anthracene oil, anthracene low.

4.3 Bioaccumulation

4.3.1 Aquatic bioaccumulation

4.3.1.1 Bioaccumulation estimation

Based on the substance's log K_{OW} range from 3.84 to 5.20, anthracene oil, anthracene low is expected to bioaccumulate.

4.3.1.2 Measured bioaccumulation data

Bioaccumulation of various PAH has been measured in various species. Several studies have been discussed in detail in the risk assessment report of anthracene (de Maagd, 1996; de Voogt *et al.*, 1991; Djomo *et al.*, 1996) and in the Annex XV transitional report for coal tar pitch, high temperature (McLeese *et al.*, 1987; Petersen and Kristensen, 1998; Bruner *et al.*, 1994). The most relevant studies and results are summarized in the following table.

Table 10: Bioaccumulation factors in fish and mollusca for the various PAHs (The Netherlands - Bureau REACH, 2009)

Substance	Species	BCF	R ^{a)}	Test system ^{b)}	Type ^{c)}	References	
Fluorene	<i>Fish</i>						
	Poecilia reticulata	2230	3	S	k1/k2 (parent)	(de Voogt <i>et al.</i> , 1991)	
	Poecilia reticulata	1050	2	R	equilibrium (parent)	(de Voogt <i>et al.</i> , 1991)	
	Poecilia reticulata	3500	2	S	equilibrium (parent)	(de Voogt <i>et al.</i> , 1991)	
Phenanthrene	<i>Fish</i>						
	Brachydanio rerio (eggs)	9120 ^{d)}	3	R	equilibrium (total = parent)	(de Voogt <i>et al.</i> , 1991)	
	Brachydanio rerio (eggs)	12303 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)	
	Brachydanio rerio (larvae)	7943 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)	
	Brachydanio rerio (larvae)	6309 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)	
	Gadus morhua (larvae)	10715 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)	
	Gadus morhua (larvae)	14454 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)	
	Clupea harengus (larvae)	20893 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)	
	Clupea harengus (larvae)	21380 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)	
	Scophthalmus maximus	11220 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)	
	Scophthalmus maximus	11482 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)	
	Brachydanio rerio	13400 ^{d)}	3	S	k1/k2 (total)	(Djomo <i>et al.</i> , 1996)	
	Pimephales promelas	6760	2	S	k1/k2 (parent)	(de Maagd, 1996)	
	Fluoranthene	<i>Mollusca</i>					
		Mytilus edulis	5920	1	F	k1/k2 (parent)	McLeese & Burrige (1987)
Mya arenaria		4120	1	F	k1/k2 (parent)	McLeese & Burrige (1987)	
<i>Fish</i>							
	Pimephales promelas	3388	2	S	k1/k2 (parent)	(de Maagd, 1996)	

Table continues on next page

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Substance	Species	BCF	Ra	Test	Type c)	References
Pyrene	<i>Mollusca</i>					
	<i>Mya arenaria</i>	6430	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	<i>Mytilus edulis</i>	4430	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	<i>Dreissena polymorpha</i>	16000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	<i>Dreissena polymorpha</i>	13000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	<i>Dreissena polymorpha</i>	35000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	<i>Fish</i>					
	<i>Brachydanio rerio</i> (eggs)	10000 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	<i>Brachydanio rerio</i> (eggs)	30200 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	<i>Brachydanio rerio</i> (larvae)	54954 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	<i>Brachydanio rerio</i> (larvae)	53703 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	<i>Gadus morhua</i> (larvae)	60256 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	<i>Gadus morhua</i> (larvae)	85114 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	<i>Clupea harengus</i> (larvae)	97724 ^{d)}	3	R	equilibrium (total = parent)	(Petersen and Kristensen, 1998)
	<i>Clupea harengus</i> (larvae)	128825 ^{d)}	3	R	k1/k2 (total = parent)	(Petersen and Kristensen, 1998)
	<i>Brachydanio rerio</i>	4300	3	S	k1/k2 (total)	(Djomo <i>et al.</i> , 1996)
	<i>Poecilia reticulata</i>	4810	3	S	k1/k2 (parent)	(de Voogt <i>et al.</i> , 1991)
	<i>Poecilia reticulata</i>	11300	2	R	equilibrium (parent)	(de Voogt <i>et al.</i> , 1991)
	<i>Poecilia reticulata</i>	2700	2	S	equilibrium (parent)	(de Voogt <i>et al.</i> , 1991)

a) Reliability score: 1-reliable without restrictions, 2-reliable with restrictions, 3-unreliable, 4-not assignable; b) S: static exposure system, F: flow-through system, R: static renewal system; c) k1/k2: uptake rate/depuration rate, total: total compound concentration (including transformation products), parent: parent compound concentration, NS, not steady state; d) based on dry weights

4.3.2 Summary and discussion of bioaccumulation

The bioaccumulation potential of anthracene has been described in the Annex XV-Dossier for identifying anthracene as a SVHC (European Chemicals Agency, 2008c). Anthracene has been placed on the Candidate List due to the identification as PBT-substance (European Chemicals Agency, 2008).

Moreover, further constituents of anthracene oil show bioaccumulation potential, too. The BCFs of fluorene, phenanthrene, fluoranthene and pyrene show values >2000 in several studies. The last 4 compounds, moreover, also fulfil the vB-criteria with BCFs >5000.

In summary, due to its constituents anthracene oil, anthracene low fulfils the B and the vB criteria according to article 57 d) and e) of the REACH regulation.

4.4 Secondary poisoning

Assessment of the potential for secondary poisoning

5 HUMAN HEALTH HAZARD ASSESSMENT

Not relevant for this dossier

6 HUMAN HEALTH HAZARD ASSESSMENT OF PHYSICO-CHEMICAL PROPERTIES

Not relevant for this dossier

7 ENVIRONMENTAL HAZARD ASSESSMENT

Anthracene oil, anthracene low consists of anthracene (>0.1%) which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008). Moreover, fluorene, phenanthrene, and pyrene belong to the 16 US-EPA PAH for which the aquatic NOEC values are < 0.01 mg/L (The Netherlands - Bureau REACH, 2009).

7.1 Aquatic compartment

7.1.1 Toxicity test results

7.1.1.1 Fish

Short-term toxicity to fish

Long-term toxicity to fish

7.1.1.2 Aquatic invertebrates

Short-term toxicity to aquatic invertebrates

Long-term toxicity to aquatic invertebrates

7.1.1.3 Algae and aquatic plants

7.1.1.4 Sediment organisms

7.1.1.5 Other aquatic organisms

7.1.2 Calculation of Predicted No Effect Concentration (PNEC)

7.1.2.1 PNEC water

7.1.2.2 PNEC sediment

7.2 Terrestrial compartment

7.2.1 Toxicity test results

7.2.1.1 Toxicity to soil macro organisms

7.2.1.2 Toxicity to terrestrial plants

7.2.1.3 Toxicity to soil micro-organisms

7.2.1.4 Toxicity to other terrestrial organisms

Toxicity to birds

Toxicity to other above ground organisms

7.2.2 Calculation of Predicted No Effect Concentration (PNEC_{soil})

7.3 Atmospheric compartment

7.4 Microbiological activity in sewage treatment systems

7.4.1 Toxicity to aquatic micro-organisms

7.4.2 PNEC for sewage treatment plant

7.5 Calculation of Predicted No Effect Concentration for secondary poisoning (PNEC_{oral})

7.6 Conclusion on the environmental classification and labelling

8 PBT, VPVB AND EQUIVALENT LEVEL OF CONCERN ASSESSMENT

8.1 Comparison with criteria from annex XIII

Anthracene oil, anthracene low is a UVCB substance consisting of a variety of different constituents. One main constituent is anthracene (1-6 %) which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d). Therefore also anthracene oil, anthracene low fulfils the PBT criteria according to Annex XIII of the REACH regulation.

Moreover, anthracene oil, anthracene low consists of further PAH which are hardly degraded. Further studies show relatively long dissipation times for fluoranthene ($\text{DisDT}_{50} > 173$ d), pyrene ($\text{DisDT}_{50} > 131$ d), and carbazole ($\text{DegDT}_{50} > 184$ d) (Grosser *et al.*, 1991; Park *et al.*, 1990). In a field study half-lives of 5.7 years for phenanthrene, 7.8 years for fluoranthene, and 8.5 years for pyrene have been measured in soil (Wild *et al.*, 1991). Therefore, anthracene-oil, anthracene low fulfils the P and the vP criteria according to Annex XIII of the REACH regulation.

In several studies conducted with different molluscs and fish species BCF values for fluorene, phenanthrene, fluoranthene and pyrene were measured > 2000 . For phenanthrene, pyrene and fluoranthene BCF values were even > 5000 (Petersen and Kristensen, 1998; McLeese *et al.*, 1987; Bruner *et al.*, 1994; de Voogt *et al.*, 1991; de Maagd, 1996; Djomo *et al.*, 1996). This means that anthracene oil, anthracene low meets the B and vB criteria according to Annex XIII of the REACH regulation.

Fluoren, phenanthrene, anthracene and pyrene belong to the 16 US-EPA PAH for which the aquatic NOEC values are < 0.01 mg/L (The Netherlands - Bureau REACH, 2009). Therefore, anthracene oil, anthracene low also meets the T criterion.

8.2 Emission characterisation

8.3 Conclusion of PBT and vPvB assessment

Anthracene oil, anthracene low is a UVCB substance consisting of a variety of different constituents. One main constituent is anthracene (1-6 %) which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d). Therefore also anthracene oil, anthracene low fulfils the PBT criteria according to Annex XIII of the REACH regulation.

Phenanthrene, fluoranthene and pyrene are present in anthracene-oil, anthracene low ($> 0.1\%$). Since these constituents fulfil the PBT and the vPvB criteria it can be concluded that anthracene oil, anthracene low meets the P, vP, B, vB and T criteria and hence is considered as a PBT and vPvB substance.

INFORMATION ON USE, EXPOSURE, ALTERNATIVES AND RISKS

1 INFORMATION ON EXPOSURE

Anthracene oil, anthracene low is mainly used as an intermediate in the production of pure anthracene, which is intensively used in the production of artificial dyes. Anthracene oil, anthracene low is also used in the following applications:

- Component in technical tar oils (e.g. for production of carbon black, heating oils, bunker fuel)
- Production of basic chemicals
- Intermediate for phyto-pharmaceutical and human-pharmaceutical products.
- Impregnation agent (mostly as wood preservative, sometimes for ropes and sailcloth)
- Component in tar paints for special application (e.g. underwater corrosion protection)
- Component of waterproof membranes for roofing and other sealing purposes
- Component of asphalt used for road construction
- Supplementary blast furnace reducing agent
- Industrial viscosity modifier

For these applications the emission to the environment is estimated to be relevant. The emission factor for the life cycle steps “use” and “service life” and the related PECs can not be assessed for these applications, because these are wide dispersive uses and the emission factor also depends on the local environmental conditions. Though, there is no information on the annual amount of anthracene oil used for these environmentally relevant applications.

CEFIC was asked to answer detailed questions concerning exposure in January 2009. An official written reply to the questionnaire was received in July after the Annex XV dossier had already been supplied to ECHA. However, only information on main uses of anthracene oils was given.

2 INFORMATION ON ALTERNATIVES

No information available

2.1 Alternative substances

2.2 Alternative techniques

3 RISK-RELATED INFORMATION

Water Framework Directive (WFD)

According to Decision 2455/2001/EC anthracene and fluoranthene are on the priority list of the Water Framework Directive 2000/60/EC. Moreover, according to the latest common position adopted by the Council, they have been identified as a “priority hazardous substances” under the WFD, which means that cessation or phasing-out of discharges, emissions and losses of anthracene and fluoranthene have to be envisaged (Common position adopted by the Council of 29th November 2007, 11486/07). As a first step in this direction environmental quality standards for anthracene and fluoranthene are proposed in the common position: the annual average concentration of anthracene and fluoranthene should not exceed 0.1 µg/l, while the maximum allowable concentration must not exceed 0.4 µg/l in inland and other surface waters.

OTHER INFORMATION

It has to be mentioned that anthracene oil, anthracene low is only one example for a number of UVCB substances containing anthracene, irrespective from their origin (e.g. from chemical coal processing or from crude oil). Anthracene is a PBT-substance. Therefore all compounds and mixtures containing anthracene need to be considered for authorization in the future, since they also fulfil the PBT criteria according to Article 57 d) of the REACH-regulation. If those UVCB substances also contain further PAH, the vPvB criteria might be fulfilled, too.

References

Calvert JG, Atkinson JR, Becker KH, Kamens RM, Seinfeld JH, Wallington TJ, Yarwood G. 2002. *The Mechanisms of Atmospheric Oxidation of Aromatic Hydrocarbons*. Oxford University Press, Oxford.

European Chemicals Agency. 2008. Support document for identification of anthracene as a substance of very high concern. ECHA, 1-27.

The Netherlands - Bureau REACH. 2009. Annex XV transitional report: coal tar pitch, high temperature (CTPHT).

Mackay D, Shiu WY, Ma K. 1992. *Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals*. Vol. II: Polynuclear aromatic hydrocarbons, polychlorinated dioxins and dibenzofurans. Lewis Publishers, Chelsea.

MITI-List. 2002. *Biodegradation and Bioaccumulation of Existing Chemical Substances under the Chemical Substance Control Law*. National Institute of Technology and Evaluation, Japan.

Coover MP, Sims RC. 1987. The Effect of Temperature on Polycyclic Aromatic Hydrocarbon Persistence in an Unacclimated Agriculture Soil. *Hazard Waste Hazard Mater* 4(1).

Wild SR, Berrow ML, Jones KC. 1991. The persistence of polynuclear aromatic hydrocarbons (PAHs) in sewage sludge amended agricultural soils. *Environ Pollut* 72:141-157.

Wild SR, Jones KC. 1993. Biological and abiotic losses of polynuclear aromatic hydrocarbons (PAH) from soils freshly amended with sewage sludge. *Environ Toxicol Chem* 12:5-12.

Grosser RJ, Warshawsky D, Vestal JR. 1991. Indigenous and Enhanced Mineralization of Pyrene, Benzo[a]pyrene, and Carbazole in Soils. *Am Soc Microbiol* 57(12):3462-3469.

Park KS, Sims RC, Dupont RR, Doucette WJ, Matthews JE. 1990 Feb. Fate of PAH compounds in two soil types: influence of volatilization, abiotic loss and biological activity. *Environ Tox Chem* 9(2):187-195.

European Chemicals Agency E. 2008. Support Document For Identification Of Anthracene As A Substance Of Very High Concern. ECHA, 1-27.

European Chemicals Agency E. 2008. Chapter R.7a: Endpoint Specific guidance. In: *Guidance On Information Requirements And Chemical Safety Assessment*. 1-428.

European Chemicals Agency E. 2008. R.16: Environmental Exposure Estimation. In: *Guidance On Information Requirements And Chemical Safety Assessment*. 1-138.

de Maagd PG-J. 1996. *Polycyclic aromatic hydrocarbons: Fate and effects in aquatic environment*. Utrecht University, Utrecht, The Netherlands.

de Voogt P, van Hattum B, Leonards P, Klamer JC, Govers H. 1991 Sep. Bioconcentration of polycyclic heteroaromatic hydrocarbons in the guppy (*Poecilia reticula*). *Aquat Toxicol* 20(3):169-194.

Djomo JE, Garrigues P, Narbonne JF. 1996. Uptake and depuration of polycyclic aromatic hydrocarbons from sediment by the zebrafish (*Brachydanio rerio*). *Environ Toxicol Chem* 15(7):1177-1181.

McLeese CW, Ray S, Burrige LE. 1987. Accumulation of polynuclear aromatic hydrocarbons by the clam *Mya arenaria*. *Wastes in the Ocean, Vol 6 - Nearshore Waste Disposal* 6:81-88.

Petersen GI, Kristensen P. 1998. Bioaccumulation of lipophilic substances in fish early life stages. *Environ Toxicol Chem* 17(7):1385-1395.

Bruner KA, Fisher SW, Landrum PF. 1994. The role of the zebra mussel, *Dreissena polymorpha*, on contaminant cycling: I. The effect of body size and lipid content on the bioconcentration of PCBs and PAHs. *J Great Lakes Res* 20(4):725-734.

European Chemicals Agency. 2008. Candidate List.