

4 December 2009

**Substance name:** Anthracene oil, anthracene-low

EC number: 292-604-8 CAS number: 90640-82-7

# MEMBER STATE COMMITTEE SUPPORT DOCUMENT FOR IDENTIFICATION OF ANTHRACENE OIL, ANTHRACENE-LOW AS A SUBSTANCE OF VERY HIGH CONCERN BECAUSE OF ITS CMR, PBT AND vPvB PROPERTIES

**Adopted on 4 December 2009** 

## **CONTENTS**

FC	)REW	ORD	3			
JU	STIFI	CATION	6			
1	IDEN	IDENTITY OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES				
	1.1	Name and other identifiers of the substance	6			
	1.2	Composition of the substance	6			
		Physico-chemical properties				
2		SSIFICATION AND LABELLING				
_						
		Classification in Annex VI of Regulation (EC) No 1272/2008				
3	ENV	TRONMENTAL FATE PROPERTIES	13			
		Degradation				
		3.1.1.1 Phototransformation	13			
		3.1.2 Biodegradation				
		3.1.2.2 Screening tests				
		3.1.2.3 Simulation tests				
		3.1.3 Summary and discussion of persistence	16			
		Environmental distribution				
		3.2.1 Adsorption/desorption				
		3.2.2 Volatilisation				
	3.3	Bioaccumulation	18			
		3.3.1.1 Bioaccumulation estimation				
		3.3.1.2 Measured bioaccumulation data				
		3.3.2 Summary and discussion of bioaccumulation	19			
4	HUM	MAN HEALTH HAZARD ASSESSMENT	19			
5	ENV	TRONMENTAL HAZARD ASSESSMENT	20			
	5.1	Aquatic compartment	20			
		5.1.1 Toxicity test results	20			
		5.1.1.1 Fish				
		5.1.1.2 Aquatic invertebrates				
6	PBT	AND VPVB ASSESSMENT				
~						
	6.1	6.1 Comparison with criteria from Annex XIII				
	6.2	Summary and overall conclusions on the PRT vPvR or equivalent level of concern properties	24			

EFERENCES	

## **TABLES**

Table 1: Summary of the physico-chemical properties of anthracene oil, anthracene-low	.10
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 as of 1 December 2010	.11
Γable 3: Classification and labelling of anthracene oil, anthracene-low according to Annex VI, part 3, Table 3.1 of	
Regulation (EC) No 1272/2008 as of 1 December 2010.	.12
Table 4: Phototransformation of the relevant constituents of anthracene oil, anthracene-low. Data were taken form	
Annex XV transitional report for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009)	.13
Table 5: Ranking of PAH in different half-life classes (The Netherlands - Bureau REACH, 2009)	.14
Table 6: Biodegradation of several PAH according to the test method MITI I (OECD TG 301C)	.14
Fable 7: Half-lives of relevant compounds present in anthracene oil	.15
Fable 8: LogK <sub>OW</sub> and logK <sub>OC</sub> data of the relevant constituents of anthracene oil, anthracene-low	.17
Fable 9: Henry constants and volatilisation of main constituents in municipal waste water treatment plants.	.17
Table 10: Bioaccumulation factors in fish and mollusca for the various PAHs (The Netherlands - Bureau REACH,	
2009)	.18
Γable 11: Examples for acute toxicity of fluoranthene to fish species	.20
Γable 12: Examples for chronic toxicity of fluoranthene to fish species. Data were taken from the Annex XV-	
ransitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009)	.21
Γable 13: Short-term toxicity to aquatic invertebrates	.21
Γable 14: Examples for chronic toxicity of pyrene and fluoranthene to aquatic invertebrates. Data were taken from	the
Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009)	.22
Table 15: Examples for chronic toxicity of pyrene and fluoranthene to algae and aquatic plants. Data were taken from	
he Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).	
Γable 16: Overview on conclusions on fulfilment of the (v)P-, (v)B- or T-criteria	24

#### **FOREWORD**

Anthracene oil, anthracene-low is an UVCB substance (substance of unknown or variable composition, complex reaction products or biological materials). It is characterised by a variable and high content of polycyclic aromatic hydrocarbons (PAHs) and heterocyclic compounds.

One relevant constituent present in anthracene oil, anthracene-low is anthracene (1-6%), which has been identified as a PBT-substance and has been placed on the Candidate List. Additionally other PAHs are present in anthracene oil, anthracene-low in individual concentrations equal to or above 0.1% (weight/weight), such as fluoranthene and pyrene.

The PBT and/or vPvB properties of the latter constituents have been discussed already in the Annex XV transitional report for coal tar pitch, high temperature and before in the Risk Assessment Report (RAR) for coal tar pitch, high temperature, indicating that the data have already been assessed for validity and relevance by a competent EU body. Therefore in the present document most data for individual PAH have been taken directly from the Annex XV transitional report and the RAR for coal tar pitch, high temperature. The data for anthracene are not discussed again in this support document, but references to the Anthracene Annex XV-Dossier are placed at appropriate positions in the text.

Substance Name: Anthracene oil, anthracene-low

EC Number: 292-604-8

CAS number: 90640-82-7

• The substance is identified as a carcinogen (category 2, R45) according to Article 57 (a) of Regulation (EC) 1907/2006 (REACH).

- The substance is identified as a mutagen (category 2, R46) according to Article 57 (b) of Regulation (EC) 1907/2006 (REACH).
- The substance is identified as a PBT according to Article 57 (d) of Regulation (EC) 1907/2006 (REACH).
- The substance is identified as a vPvB according to Article 57 (e) of Regulation (EC) 1907/2006 (REACH).

# 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 PAHs such as fluoranthene (5-15%) and pyrene (2-8%), which fulfil both the PBT and vPvB criteria. The constituent phenanthrene (10-30 %) fulfils the vPvB criteria.

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

According to Annex VI, part 3, Table 3.2 of Regulation (EC) No 1272/2008¹ the classification as carcinogen (Carc. Cat.2, R45)² must be applied to anthracene oil, anthracene-low unless it can be shown that the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7) and less than 0.005 % w/w benzo[a]pyrene (EINECS No 200-028-5).

Pursuant to Annex IV of Commission Regulation (EC) No 790/2009<sup>3</sup> as of 1 December 2010 the classification as mutagen (Muta. Cat.2; R46) must be applied to anthracene oil, anthracene-low unless the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7).<sup>4</sup>

<sup>1</sup> Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

<sup>&</sup>lt;sup>2</sup> This corresponds to a classification Carc. 1B; H350 in Annex VI, part 3, Table 3.1 of Regulation (EC) No 1272/2008.

<sup>&</sup>lt;sup>3</sup> Commission Regulation (EC) No 790/2009 of 10 August 2009 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures (1<sup>st</sup> ATP)

Hence, anthracene oil, anthracene-low is a substance meeting the criteria for identification as a carcinogen and mutagen according to Article 57(a) and 57 (b) of the REACH Regulation where the conditions for its classification have been met.

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

Not available.

 $<sup>^4</sup>$  Pursuant to the  $1^{\rm st}$  ATP, the classification according to Table 3.1 of Annex VI, part 3, of Regulation (EC) No 1272/2008 will as of 1 December 2010 be mutagen category 1B, H340..

#### **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 derivates 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:

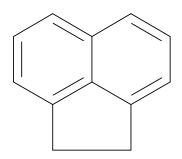
Chemical Name: Acenaphthene EC Number: 201-469-6

CAS Number: 83-32-9

IUPAC Name: 1,2-dihydroacenaphthylene

Molecular Formula: C12H10

Structural Formula:



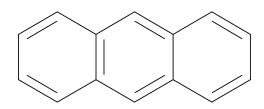
Molecular Weight: 154.21

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):

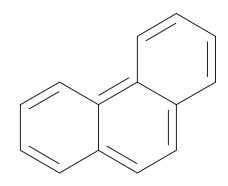
Concentration range (% w/w): 1 - 6

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

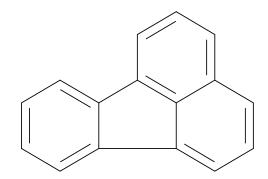
Chemical Name: Fluoranthene

EC Number: 205-912-4 CAS Number: 206-44-0

IUPAC Name: Fluoranthene

Molecular Formula: C16H10

Structural Formula:



Molecular Weight: 202.26

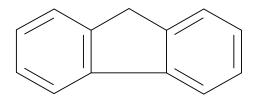
Typical concentration (% w/w):

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:



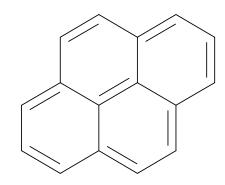
Molecular Weight: 166.22

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: 9*H*-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 of anthracene oil, anthracene-low

REACH ref Annex, §	Property	IUCLID section	Value	Comment/reference
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 CLASSIFICATION AND LABELLING

#### 2.1 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<sup>5</sup>.

Its classification has been updated under the same index number in Annex IV of Commission Regulation (EC) No 790/2009<sup>6</sup>. Classification as mutagen (Muta. Cat.2; R 46) has been added.

Pursuant to Annex IV of Commission Regulation (EC) No 790/2009 anthracene oil, anthracene-low will as of 1 December 2010 be listed in Table 3.2 (the list of harmonised classification and labelling of hazardous substances from Annex I to Directive 67/548/EEC) of Annex VI, part 3, of Regulation (EC) No 1272/2008 as shown 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 as of 1 December 2010

Name	CAS-No	Index-No	Classification	Labelling	Notes
Anthracene oil, anthracene-low	90640-82-7	648-104-00-0	Carc. Cat 2; R45 Muta. Cat.2; R46	T; R45-46; S 53 – 45	НЈМ

#### Notes:

**H:** 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.

*J:* The classification as a carcinogen or mutagen need not apply if it can be shown that the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7).

**M:** 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-low as hazardous substance according to Regulation (EC) No 1272/2008 (Annex VI, part 3, Table 3.1 (the list of harmonised classification and labelling of hazardous substances)) as of 1 December 2010 is provided in Table 3.

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<sup>&</sup>lt;sup>5</sup> Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures, amending and repealing Directives 67/548/EEC and 1999/45/EC, and amending Regulation (EC) No 1907/2006.

<sup>&</sup>lt;sup>6</sup> Commission Regulation (EC) No 790/2009 of 10 August 2009 amending, for the purposes of its adaptation to technical and scientific progress, Regulation (EC) No 1272/2008 of the of the European Parliament and of the Council on classification, labelling and packaging of substances and mixtures (1<sup>st</sup> ATP)

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 as of 1 December 2010.

Name	CAS-No	Index-No	Classification	Labelling	Notes
Anthracene oil, anthracene-low	90640-82-7	648-104-00-0	Carc. Cat 1B H350 Muta. Cat. 1B H340	GHS08 Dgr H350 H340	НЈМ

#### Notes:

**H:** 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 for manufacturers, importers or downstream users of this substance apply to all other hazard classes and categories. For hazard classes where the route of exposure or the nature of the effects leads to a differentiation of the classification of the hazard class, the manufacturer, importer or downstream user is required to consider the routes of exposure or the nature of the effects not already considered.

*J:* The classification as a carcinogen or mutagen need not apply if it can be shown that the substance contains less than 0.1 % w/w benzene (EINECS No 200-753-7).

**M:** 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).

#### 3 ENVIRONMENTAL FATE PROPERTIES

#### 3.1 Degradation

#### 3.1.1 Stability

#### 3.1.1.1 Phototransformation

Photolysis in the troposphere results in the formation of reactive hydroxyl (OH) and nitrate (NO<sub>3</sub>) radicals and ozone (O<sub>3</sub>), which react as oxidising agents with organic compounds like PAHs. Reactions with these radicals and ozone reactions comprise the main degradation path of gas-phase PAH (Calvert et al., 2002). The atmospheric behaviour of the main constituent of anthracene oil, anthracene-low is shown below in Table 4.

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

	Representative lifetime in air with respect to reaction with					
PAH (number of rings)		ОН	NO <sub>3</sub>	$O_3$		
	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 support document with AOPwin v1.91.

For all these substances the transformation rate in particle phase is expected to be slower. Particle phase transformation is, however, not assumed to be of relevance for the overall atmospheric lifetime, because only up to 3% of atmospheric anthracene, 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.

#### 3.1.1.2 Hydrolysis

Hydrolysis as a way of abiotic degradation can be considered as not relevant for the main constituents of the UVCB substance anthracene oil, anthracene-low because of their chemical structures. 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 (MITI-List, 2002).

#### 3.1.2 Biodegradation

#### 3.1.2.1 Biodegradation estimation

The PAH listed in Table 5 were allocated to persistence classes on the basis of model calculations (Mackay et al., 1992). These half-lives were used 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 (The Netherlands - Bureau REACH, 2009)

Substance	Water		Soil		Sediment	
	class	Half-life [d]	class	Half-life [d]	class	Half-life [d]
Acenaphtene	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

#### 3.1.2.2 Screening tests

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

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

Compound	BOD	Judgement
Phenanthrene	54 %	not-readily biodegradable
Fluorene	0 %	not-readily biodegradable
Carbazole	0 %	not-readily biodegradable
Acenaphthene	0%	not-readily 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 elimination increased. 19% (2%) of phenanthrene, 71% (15%) of fluoranthene and 89% (43%) of pyrene were remaining at 20°C (30°C).

#### 3.1.2.3 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 revealed 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. (1991) studied the mineralisation of <sup>14</sup>C-labelled pyrene and carbazole in three different soils. The mineralisation 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 mineralisation 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 was testes by (Park et al., 1990). The half-life of phenanthrene was calculated as being in the range of 27 and 53 days (second soil: 13 - 18 days), whereas the half life of fluoranthene ranged between 173 and 630 days (second soil: 277 - 578 days) and that of pyrene between 131 and 408 days (second soil: 193 - 408 days).

Table 7. IIak kana	-f11-	
Table /: Half-lives	of relevant compounds	present in anthracene oil

Substance	Result	Reference
Phenanthrene	$DisDT_{50} = 5.7$ years (field study)	(Wild et al., 1991)
	DisDT <sub>50</sub> =83 – 193 d (microcosm study)	(Wild and Jones, 1993)
	Elimination half- life in two different soils:	(Park et al., 1990)
	DisDT <sub>50</sub> = $27 - 53 \text{ d}$	
	$DisDT_{50} = 13 - 18 d$	
Fluoranthene	$DisDT_{50} = 7.8$ years (field study)	(Wild et al., 1991)

	DisDT <sub>50</sub> = $110 - 184$ d (microcosm study)				
	Elimination half- life in two different soils: $DisDT_{50} = 173 - 630 d$	(Park et al., 1990)			
	$DisDT_{50} = 277 - 578 d$				
Pyrene	Degradation half-life:	(Grosser et al.,			
	$DegDT_{50} > 184 d (10 - 48 \% mineralization in 184 d)$	1991)			
	(Wild et al., 1991)				
	(Wild and Jones, 1993)				
	Elimination half- life in two different soils:	(Park et al., 1990)			
	$DisDT_{50} = 131 - 408 d$				
	$DisDT_{50} = 193 - 408 d$				
Carbazole	azole Degradation half-life:				
	$DegDT_{50} > 184 d$ (undetectable – 46 % mineralisation in				

#### 3.1.3 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, 2008e).

Moreover, anthracene oil, anthracene-low consists of further not readily degradable PAH constituents. Model calculations by Mackay et al. (1992) indicate that acenaphtene, fluorene, phenanthrene, fluoranthene, and pyrene show half-life in sediment of more than 180 days.

Screening studies (OECD TG 301C) revealed, that phenanthrene, acenaphtene, fluorene and carbazole as representative constituents in anthracene oil, anthracene-low are not readily biodegradable (MITI-List, 2002).

Further studies showed relatively long dissipation times for fluoranthene (DisDT<sub>50</sub> > 173 d), pyrene (DisDT<sub>50</sub> > 131 d), and carbazole (DegDT<sub>50</sub> > 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, anthracene-low fulfil the P or the vP criteria of Annex XIII of the REACH regulation.

#### 3.2 Environmental distribution

#### 3.2.1 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, 2008c). The results are shown below in Table 8.

Table 8:  $LogK_{OW}$  and  $logK_{OC}$  data of the relevant constituents of anthracene oil, anthracene low.

Substance	CAS-No.	logK <sub>OW</sub> a)	log K <sub>OC</sub>	$K_{OC}$ (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 were 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.

#### 3.2.2 Volatilisation

For the substance anthracene oil, anthracene-low no measured data are available at the moment. According to the constituents' Henry's Law constants anthracene oil, anthracene-low is expected 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).

#### 3.2.3 Distribution modelling

For the main constituents of anthracene oil the behaviour in the wastewater treatment plant was calculated under the assumption that no biodegradation occured (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 <sup>a</sup>	Distribution of PAH in STP <sup>b</sup>					
	(Pa*m³/mol)	% 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

<sup>&</sup>lt;sup>a</sup> calculation of Henry's Law coefficient according to Guidance document R.16 (European Chemicals Agency, 2008d); <sup>b</sup> 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.

#### 3.3 Bioaccumulation

#### 3.3.1 Aquatic bioaccumulation

#### 3.3.1.1 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.

#### 3.3.1.2 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 Voogt et al., 1991; Djomo et al., 1996; de Maagd, 1996) and in the Annex XV transitional report for coal tar pitch, high temperature (McLeese et al., 1987; Bruner et al., 1994; Petersen and Kristensen, 1998). The most relevant studies and results are summarised in Table 10.

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

Substance	Species	BCF	R <sup>a)</sup>	Test system b)	Type c)	References
Fluorene	Fish					
	Poecilia reticulata	2230	3	S	k1/k2 (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	1050	2	R	equilibrium (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	3500	2	S	equilibrium (parent)	(de Voogt et al., 1991)
Phenanthrene	Mollusca					
	Mytilus edulis	1240	1	F	k1/k2	(McLeese et al., 1987)
	Mya arenaria	1280	1	F	k1/k2	(McLeese et al., 1987)
	Fish					
	Cyprinodon variegatus	810 <sup>d)</sup>	1	F	k1/k2 (parent)	(Jonsson et al., 2004)
	Cyprinodon variegatus	2229 <sup>e)</sup>	1	F	k1/k2 (parent)	(Jonsson et al., 2004)
	Cyprinodon variegatus	700 <sup>d)</sup>	1	F	equilibrium (parent)	(Jonsson et al., 2004)
	Cyprinodon variegatus	1623 <sup>e)</sup>	1	F	equilibrium (parent)	(Jonsson et al., 2004)

	Pimephales promelas	6760	2	S	k1/k2 (parent)	(de Maagd, 1996)
Fluoranthene	Mollusca					
	Mytilus edulis	5920	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Mya arenaria	4120	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Fish					
	Pimephales promelas	3388	2	S	k1/k2 (parent)	(de Maagd, 1996)
Pyrene	Mollusca					
	Mya arenaria	6430	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Mytilus edulis	4430	1	F	k1/k2 (parent)	McLeese & Burridge (1987)
	Dreissena polymorpha	16000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	Dreissena polymorpha	13000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	Dreissena polymorpha	35000	2	S	k1/k2 (total = parent)	(Bruner et al., 1994)
	Fish					
	Poecilia reticulata	11300	2	R	equilibrium (parent)	(de Voogt et al., 1991)
	Poecilia reticulata	2700	2	S	equilibrium (parent)	(de Voogt et al., 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) low exposure concentration; e) high exposure concentration.

#### 3.3.2 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, 2008a).

Moreover, further constituents of anthracene oil, anthracene-low show bioaccumulation potential, too. The BCF of fluorene, phenanthrene, fluoranthene and pyrene have shown to be >2000 in several studies. The last three constituents, additionally, fulfil the vB-criteria with BCFs >5000.

In summary, several constituents of anthracene oil, anthracene-low fulfil the B or the vB criteria of Annex XIII of the REACH regulation.

#### 4 HUMAN HEALTH HAZARD ASSESSMENT

Not considered in this document.

#### 5 ENVIRONMENTAL HAZARD ASSESSMENT

#### 5.1 Aquatic compartment

One constituent of anthracene oil, anthracene-low is anthracene, which has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008b). Therefore, the toxicity data of this substance are not presented again. Fluoranthene and pyrene, which are also present in anthracene oil, anthracene-low are also toxic to aquatic organisms.

Exposure to PAH (such as anthracene, fluoranthene and pyrene) under UV-radiation enhances the ecotoxicity of several PAH, i.a., in fish, invertebrates and algae (The Netherlands - Bureau REACH, 2009). The mechanism of photo-enhanced toxicity is not fully understood. Enhanced effects have been attained already with very short exposures to natural sunlight or UV-light (0.5 to 6 hours) and with light intensities corresponding to conditions in several meters depth of natural waters. Hence, photo-enhanced toxicity is considered a relevant phenomenon in the environment.

The most reliable study with the most sensitive organism for the evaluation of the toxicity of fluoranthene was published by (Spehar et al., 1999). It has been shown that ultraviolet (UV) light increases the acute toxicity of fluoranthene (Spehar et al., 1999). For pyrene two studies as an example for the toxicity were selected and described in the following tables (Lyons et al. 2002 and Pelletier et al. 1997).

Available studies on the toxicity to fish, invertebrates and algae are described in detail in the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009). The most reliable acute and chronic toxicity data for fish, invertebrates and algae are listed in Tables 11 to 15.

#### 5.1.1 Toxicity test results

#### 5.1.1.1 Fish

Short-term toxicity to fish

Table 11: Examples for acute toxicity of fluoranthene to fish species

Substance	Species	Exposure duration	End- point	Effect	Conc. (mg/L)	Ref.
Fluoranthene	Pseudopleuronecte s Americanus (winter flounder)	96 h	LC <sub>50</sub>	Mortality	0.0001*	(Spehar et al., 1999)
	Pseudopleuronecte s americanus (winter flounder)	96 h	LC <sub>50</sub>	Mortality	> 0.188#	(Spehar et al., 1999)

<sup>\*</sup>UV light exposure; # fluorescent light

Acute toxicity data for pyrene on fish are not available.

Long-term toxicity to fish

Table 12: Examples for chronic toxicity of fluoranthene to fish species. Data were taken from the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Substance	Species	Exposure duration	Endpoi nt	Effect	Conc. (mg/L)	Referen ce
Fluoranthene	Pimephales promelas	32 d	NOEC	ELS	0.0014	(Spehar et al., 1999)
	Pimephales promelas	11w	NOEC	Survival of hatchling s	< 0.0062	(Diamon d et al., 1995)

Chronic toxicity data for pyrene on fish are not available.

#### **5.1.1.2** Aquatic invertebrates

#### **Short-term toxicity to aquatic invertebrates**

Table 13: Short-term toxicity to aquatic invertebrates

Substance	Species	Exposure duration	End- point	Effect	Conc. (mg/L)	Ref.
Fluoranthene	Americamysis bahia (reported as Mysidopsis bahia)	96 h	LC50	Mortality	0.0014	(Spehar et al., 1999)
	Americamysis bahia (reported as Mysidopsis bahia)	96 h	LC50	Mortality	0.031#	(Spehar et al., 1999)
Pyrene	Mulinia lateralis (Dwarf Surf Clam)	48 h	EC50	Bivalve embryo response	0.0002 3*	(Pelletier et al., 1997)
	Mulinia lateralis (Dwarf Surf Clam)	96 h	LC50	Mortality	0.0016 8*	(Pelletier et al., 1997)
	Crassostrea gigas (Pacific oyster)	48 h	NOEC	Develop- mental success	0.0005	(Lyons et al., 2002)

<sup>\*</sup>UV light exposure; \* fluorescent light; a bivalve embryo response: Embryo/larval bivalve survival and development was determined by counting the number of normal larvae per millilitre in each replicate. Bivalve embryo/ larval survival and development is later referred to as bivalve embryo response.

#### Long-term toxicity to aquatic invertebrates

Table 14: Examples for chronic toxicity of pyrene and fluoranthene to aquatic invertebrates. Data were taken from the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Substance	Species	Exposure duration	End- point	Effect	Conc. (mg/L)	Ref.
Pyrene	Crassostrea gigas	48 h	NOEC	Shell develop ment	0.0005	(Lyons et al., 2002)
	Ceriodaphnia dubia	7 d	EC10	Reproduc tion	0.0021	(Bisson et al., 2000)
Fluoranthene	Mysidopsis bahia	31 d	NOEC	Reproduc tion	0.0006	(Spehar et al., 1999)
	Daphnia magna	21 d	NOEC	Growth	0.0014	(Spehar et al., 1999)

<sup>\*</sup>UV light exposure

#### 5.1.1.3 Algae and aquatic plants

Table 15: Examples for chronic toxicity of pyrene and fluoranthene to algae and aquatic plants. Data were taken from the Annex XV-transitional dossier for coal tar pitch, high temperature (The Netherlands - Bureau REACH, 2009).

Substance	Species	Exposure duration	End- point	Effect	Conc. (mg/L)	Ref.
Pyrene	Pseudokirchnerie lla subcapitata	72 h	EC10	Growth	0.0012	(Bisso n et al., 2000)
Fluoranthene	Pseudokirchnerie lla subcapitata	72 h	EC10	Growth	0.0086	(Bisso n et al., 2000)

#### 6 PBT AND VPVB ASSESSMENT

#### 6.1 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 also fulfil the criteria of Annex XIII:

#### Fluoranthene:

In a field study a half-live of 7.8 years for fluoranthene has been measured in soil (Wild et al., 1991). Several other studies show relatively long dissipation times for fluoranthene (DisDT $_{50} > 173$  d) in different soils (Park et al., 1990; Grosser et al., 1991). Therefore, the P and the vP criteria are fulfilled.

In studies conducted with different mollusc species BCF values > 5000 (3388 to 5920) have been measured (McLeese et Burridge, 1987 de Maagd, 1996). This means that the B and the vB criteria are fulfilled, too.

Additionally, the long-term aquatic NOECs of fluoranthene are in the range from 0.0014 to 0.0006 mg/l (Spehar et al., 1999). Therefore also the T criterion is fulfilled.

#### Pyrene:

In a field study a half-live of 8.5 years for pyrene has been measured in soil (Wild et al., 1991). Several other studies show relatively long dissipation times for pyrene (DisDT $_{50} > 131$  d) in different soils (Park et al., 1990; Grosser et al., 1991). Therefore, the P and the vP criteria are fulfilled.

In several studies conducted with different mollusc and fish species BCF values > 5000 were measured (McLeese et Burridge, 1987; de Voogt et al., 1991). This means both the B and the vB criteria are fulfilled, too.

Additionally, the aquatic NOECs of pyrene are below 0.01 mg/l. Chronic values for fish are not available, but NOECs fo aquatic invertebrates are as low as 0.0005 mg/l (shell development, *Crassostrea gigas*, Lyons et al., 2002). Therefore also the T criterion is fulfilled.

#### Phenanthrene:

In a field study a half-live of 5.7 year for phenanthrene, has been measured in soil (Wild et al., 1991). Therefore, the P and the vP criteria are fulfilled.

In one study conducted with fish (Pimephales promelas) a BCF value > 5000 was measured (de Maagd, 1996). This means that the B and the vB criteria are fulfilled, too.

# 6.2 Summary and overall conclusions on the PBT, vPvB or equivalent level of concern properties

In accordance with the guidance available for assessment of multi-constituent and UVCB substances, the PBT assessment for anthracene oil, anthracene-low focuses on the assessment of its PAH-constituents present in concentrations  $\geq 0.1\%^7$  such as anthracene (presence 1-6%), fluoranthene (5-15%), pyrene (2-8%) and phenanthrene (10-30%). Anthracene has already been identified as PBT-substance and has been added to the Candidate List (European Chemicals Agency, 2008d).

An overview on the conclusions drawn on persistence, potential for bioaccumulation and toxicity to human health and/or the environment based on comparison of the data presented for four indicator PAH-constituents of anthracene oil, anthracene-low with the PBT/vPvB criteria of Annex XIII of the REACH Regulation is provided in Table 16.

Table 16: Overview on conclusions on fulfilment of the $(v)P$ -, $(v)B$ - or T-criteria of Annex XIII of the REACH Regulation for the four indicator PAH-constituents of anthracene oil, anthracene-low								
Substance Persistence Bioaccu- mulation Toxicity Toxicity Human Aquatic Conclusion health Environment								
Anthracene	vP	В	-	T	PBT			
Phenanthrene	vP	vB	-	-	vPvB			
Fluoranthene	vP	vB	-	T	PBT/vPvB			
Pyrene	vP	vB	-	T	PBT/vPvB			

Based on the data available, it is concluded that two PAH-constituents present in anthracene oil, anthracene-low in concentrations equal to or above 0.1% are to be considered as both vPvB and PBT substances. These are fluoranthene and pyrene.

Phenanthrene fulfils the vPvB criteria, but not the PBT criteria. Anthracene fulfils the PBT criteria, but not the vPvB criteria.

In summary, anthracene oil, anthracene-low needs to be considered as a substance with both vPvB and PBT properties because of the above conclusions on the vPvB and PBT properties of its constituents anthracene, fluoranthene, pyrene and phenanthrene. It is concluded that anthracene oil, anthracene-low is a substance containing at least 18% of PAH-constituents with vPvB and/or PBT properties.

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<sup>&</sup>lt;sup>7</sup> Chapter R.11 (PBT assessment) of the guidance on information requirements and chemical safety assessment (ECHA)

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