TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

RESULTS OF THE EVALUATION OF THE PBT/VPVB PROPERTIES OF:

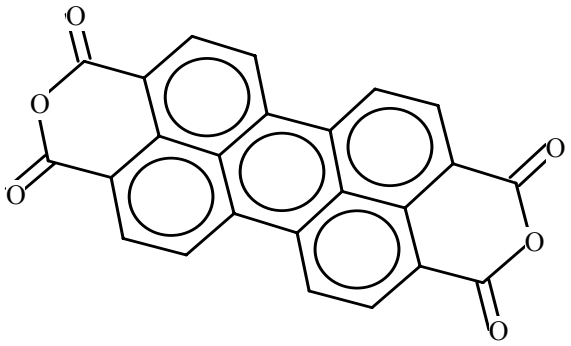
Substance name: perylene-3,4:9,10-tetracarboxylic dianhydride

EC number: 204-905-3

CAS number: 128-69-8

Molecular formula: C24H8O6

Structural formula:



Summary of the evaluation:

Perylene-3,4:9,10-tetracarboxylic dianhydride is not considered as a PBT substance. Perylene-3,4:9,10-tetracarboxylic dianhydride meets the P/vP criteria based on screening data but it does not fulfil the screening B criterion. The substance is hydrolysed (probably with a very slow rate) to perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3). This acid meets the P/vP criteria but not the B criterion both according to screening data. Ecotoxicity was not evaluated for this report.

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: perylene-3,4:9,10-tetracarboxylic dianhydride
EC Number: 204-905-3
CAS Number: 128-69-8
IUPAC Name:
Molecular Formula: C24H8O6
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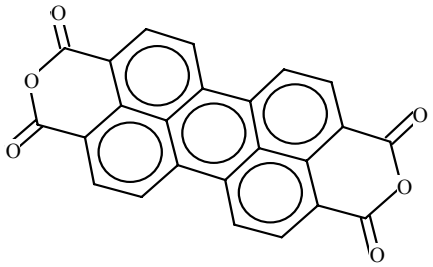


Molecular Weight: 392.33
Synonyms: C.I.Pigment Red 224; CI 71127

1.1 PURITY/IMPURITIES/ADDITIVES

No additives, may contain small amounts of impurities (at least perylene-3,4:9,10-tetracarboxylic acid) (BASF, 2004a).

1.2 PHYSICO-CHEMICAL PROPERTIES

Table 1 Summary of physico-chemical properties

REACH ref Annex, §	Property	Value	Comments
V, 5.1	Physical state at 20 C and 101.3 kPa	solid	
V, 5.2	Melting / freezing point	> 340°C	HOECHST (1988)
V, 5.3	Boiling point	-	
V, 5.5	Vapour pressure	-	
V, 5.7	Water solubility	< 0.005 mg l^{-1} at 25°C at pH 4	BASF AG (2004a)
		< 0.005 mg l^{-1} at 25°C in demineralised water	BASF AG (2004a)
		< 1 mg l^{-1} at 20°C (pH 4, 7, 9 and 12)	BASF AG (2003a)
		0.0012 mg l^{-1} at 25°C	WSKOW v1.41
		0.130 mg l^{-1}	ACD/I-LAB Web service (2003)
V, 5.8	Partition coefficient n-octanol/water (log value)	6.26	KOWWIN v1.41
VII, 5.19	Dissociation constant	-	

The water solubility limits of 5 µg l^{-1} obtained in a study resembling OECD 105 (BASF AG, 2004a) should be regarded as the maximum possible level of solubility for the substance. The value covers the error range based on all found individual values of all tests performed with a series of amounts of test substance. It is noted that the sensitivity was in this study probably limited by the direct detection of the substance in the test solutions with fluorescence spectroscopy. The sensitivity could have been enhanced by concentrating the substance with a proper extraction method before analysis.

According to BASF AG (2004a,b) results, perylene-3,4:9,10-tetracarboxylic dianhydride and its impurities and/or reaction products dissolve into distilled water at levels of 30-50 µg l^{-1} and the proportion of the substance itself is < 5 µg l^{-1}. Further measurements were carried out using the spectra of colloidal dissolved perylene-3,4:9,10-tetracarboxylic dianhydride and the results were compared with solid state spectra. Fluorescent spectra were analysed and the deviations from the solid state spectra were interpreted as soluble fraction The total soluble fraction was this way determined to be ca. 40 µg l^{-1} (including impurity and/or hydrolysed dianhydride). All measurements were influenced by the reactivity of perylene-3,4:9,10-tetracarboxylic dianhydride.

The molecular size is according to the calculations of the Rapporteur using ACD-Labs 3d –program 16 · 9 · 3.5 $Å^3$.

Octanol solubility was determined at < 1 mg l^{-1} (60 ± 30 µg l^{-1}at 25°C) by BASF (2004a). The applied method was OECD 105 and analytical determination occurred with fluorescence spectrometry.

Water solubility of the hydrolysis product perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3) is 2,6 g l^{-1} (pH 12) and < 1 mg l^{-1} in octanol (method UV/VIS spectrometry)(BASF (2004a). The hydrolysis product has calculated pKa (1-4) values of 2.36, 2.94, 3.77, 4.35 (ACD/I-Lab Web service, 2003). Based on the estimated pKa-values, the substance is present in environmentally

relevant pH range (ca. 4-9) in ionised form each of the molecule being either fully or partly ionised (note: four carboxylic acid groups).

2 MANUFACTURE AND USES

Two companies have provided information on the substance under Regulation 93/793/EEC. The total annual average EU consumption volume is expected to be between 100-1000 t/a. The majority of the produced volume is used according to industry as an on-site and/or off-site intermediate in production of perylene pigments.

3 CLASSIFICATION AND LABELLING

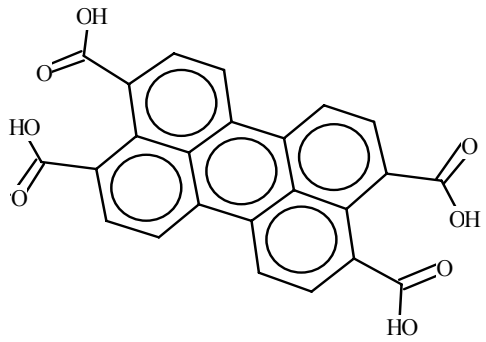
The substance is not classified under Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 DEGRADATION (P)

4.1.1 Abiotic degradation

The substance hydrolyses very slowly, whereas the rate could be assumed to be limited also by dissolution based on modified standard water solubility and accompanying stability tests of (BASF AG, 2003a and 2004a,b). The substance was observed to react in the tests with the buffer forming slightly more soluble products. The reaction was absent or negligible at pH 4 and in demineralised water but occurred fast in buffered test solutions at pH ≥ 7. It is not possible to deduce a hydrolysis rate from the available tests, but they provide clear evidence that hydrolysis is occurring in the environmentally relevant pH range. However, it is very likely, that the hydrolysis in the environment is very slow. The (stable) hydrolysis product is based on information on the group of anhydrides expected to be perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3; see structural formula below).



Indirect photochemical degradation in the atmosphere is considered to be slow based on the estimated half-life of 2.2 days for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; 5*10^5

OH^{-} cm^{-3}). It must be, however, noted, that this substance is not expected to be found in air due to its other properties.

4.1.2 Biotic degradation

No experimental data on biodegradation are available for the substance. QSAR-estimates for the substance and its hydrolysis product are presented in **Table 4.1**.

Table 4.1 BIOWIN v4.02 estimates of perylene-3,4:9,10-tetracarboxylic dianhydride and perylene-3,4:9,10-tetracarboxylic acid

	BIOWIN 2 v4.02	BIOWIN 3 v4.02	BIOWIN 6 v4.02
Perylene-3,4:9,10-tetracarboxylic dianhydride	0.00	1.53	0.00
Perylene-3,4:9,10-tetracarboxylic acid	0.02	1.80	0.71

4.1.3 Other information [1]

No data available.

4.1.4 Summary and discussion of persistence

According to the observations made in the available (modified) standard water solubility and accompanying stability tests, (BASF AG, 2003a; 2004a,b), it can be concluded that the substance hydrolyses under environmentally relevant pH but no judgement about the rate of hydrolysis can be done. It is however likely, that hydrolysis is not a significant route of degradation for the substance as the very low water solubility would be one relevant limiting factor for the hydrolysis. The stable hydrolysis product is expected to be perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3).

No experimental data on biodegradation of the substance or its acid are available. According to the BIOWIN-estimates, both substances seem potentially persistent.

4.2 ENVIRONMENTAL DISTRIBUTION

Data not reviewed for this report.

4.2.1 Adsorption

4.2.2 Volatilisation

4.2.3 Long-range environmental transport

[1] For example, half life from field studies or monitoring data

4.3 BIOACCUMULATION (B)

4.3.1 Screening data

Using the estimated logKow of 6.26, a BCF of 13,000 has been estimated for perylene-3,4:9,10-tetracarboxylic dianhydride using BCFWIN v2.15. Perylene-3,4:9,10-tetracarboxylic dianhydride has a very low octanol solubility (60 ± 30 µg l^{-1}, BASF, 2004a). Such a low octanol solubility is expected to limit the uptake of the substance by biota. For substances with a low octanol solubility, logKow is not a good predictor of bioaccumulation potential.

For the hydrolysis product perylene-3,4:9,10-tetracarboxylic acid a BCF of 5.6 has been estimated with BCFWIN v2.15 (log Kow of 5.63 used). The value provided by BCFWIN is applicable for almost all ionic substances with a logKow between 5 and 6. The low BCF for the hydrolysis product is predicted, while the substance is according to its pKa-values present in its ionic (carboxylate) form in the environment. A direct prediction of the bioaccumulation potential from logKow is not well applicable for substances present in the environment in ionised form. However, due to the predicted BCF and the high degree of ionisation, it is concluded that the hydrolysis product is expected to have a low bioaccumulation potential in the environment.

4.3.2 Measured bioaccumulation data

No experimentally derived BCF is available for the substance or its hydrolysis product.

4.3.3 Other supporting information[2]

No data available.

4.3.4 Summary and discussion of bioaccumulation

No experimental data on bioaccumulation are available for the substance or its hydrolysis product. Perylene-3,4:9,10-tetracarboxylic dianhydride is not likely to bioaccumulate in biota due to its very low octanol solubility. The estimated logKow is for this substance not a good predictor of bioaccumulation.

The slowly forming hydrolysis product perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3) is present in the environmentally relevant pH range (4-9) solely in ionised form (either all or part of the four carboxylic acid fragments are ionised depending on the pH). The logKow of 5.63 for the unionised form is not a good predictor of bioaccumulation for the ionised form. The BCF estimated for this acid is 5.6. It is concluded that due to the low predicted BCF and the high degree of ionisation, the hydrolysis product is not expected to accumulate in biota.

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

[2]For example, measured concentrations in biota

6 ENVIRONMENTAL HAZARD ASSESSMENT

No experimental data are available for the substance. QSAR-models are not well applicable for this substance due to its very low octanol solubility.

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

6.1.1 Toxicity test results

6.1.1.1 Fish

Acute toxicity

Long-term toxicity

6.1.1.2 Aquatic invertebrates

Acute toxicity

Long-term toxicity

6.1.1.3 Algae and aquatic plants

6.1.2 Sediment organisms

6.1.3 Other aquatic organisms

6.2 TERRESTRIAL COMPARTMENT

6.3 ATMOSPHERIC COMPARTMENT

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Perylene-3,4:9,10-tetracarboxylic dianhydride is hydrolysed under environmentally relevant pH range. However, the rate of hydrolysis cannot be judged based on available data and but it is likely to be slow due to the very low water solubility of the parent substance. The hydrolysis product is expected to be perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3). The parent substance and its hydrolysis product fulfil according to BIOWIN –models the criteria of potentially persistent substances. It is concluded that the substance and its (probably slowly forming) hydrolysis product are considered as meeting the P/vP criteria according to screening data.

Bioaccumulation: The substance has a very low octanol solubility (0.06 mg l^{-1}). This value is approximately 10 times lower than the octanol solubility screening trigger for the substance ($0.002 \cdot MW = 0.785$ mg l^{-1}; baseline toxicity assumed). Hence, it is concluded that the substance is not fulfilling the B criterion based on screening data. The predicted logKow of the hydrolysis product perylene-3,4:9,10-tetracarboxylic acid is 5.63 for the unionised form. However, logKow for unionised form is not a good predictor of bioaccumulation potential of the substance due to the fact, that it is present in environmentally relevant pH-range in ionised form. Based on the estimated BCF of 5.6, which has been predicted for the substance by BIOWIN v4.02, and due to its high degree of ionisation, the hydrolysis product is concluded to not to fulfil the B criterion according to screening data.

Toxicity: No experimental ecotoxicity data are available for the substance. Ecotoxicity of the substance was not evaluated for this report.

Summary: Perylene-3,4:9,10-tetracarboxylic dianhydride meets the P/vP criteria based on screening data but it does not fulfil the screening B criterion. The substance is hydrolysed (probably with a very slow rate) to perylene-3,4:9,10-tetracarboxylic acid (CAS 81-32-3). This acid meets the P/vP criteria but not the B criterion both according to screening data. Ecotoxicity was not evaluated for this report. It is concluded that perylene-3,4:9,10-tetracarboxylic dianhydride is not considered as a PBT substance.

INFORMATION ON USE AND EXPOSURE

Not relevant as the substance is not identified as a PBT.

OTHER INFORMATION

The information and references used in this report were taken from the following sources:

ACD/I-Lab Web service (2003) Aqueous solubility (v7.04) and pKa online calculation models.

BASF AG (2004a) GKA Competence Center Analytics, study 04E01503, 26 Determination of the solubility of perylen-3,4,9,10 –tetracarboxylic dianhydride in water and in octanol. 26-Apr 2004.

BASF AG (2004b) GKA Competence Center Analytics, study 04E05144, Investigations on the stability of perylen-3,4,9,10 –tetracarboxylic dianhydride in demineralized water and in buffer solutions at pH 7 and pH 8 over different time periods, 11-Aug-2004.

BASF AG (2003a) A Letter/pdf-document from BASF AG. 13. Oct. 2003 to the FIN rapporteur. Including: “Water solubility of “Persäure” at pH 4, 7, 9 and 12, GKA Competence Center Analytics, Study no. 03L00154,

BASF AG (2003b) ECB list of potential PBT/vPvB substances – perylene-3,4:9,10-tetracarboxylic dianhydride (CAS No. 128-69-8), letter 16.5.2003.

HOECHST (1988) Persäure, Prüfung der akuten Toxizität am Fisch Zebrabärbling (*Brachydanio rerio)* über 96 stunden.