TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVB SUBSTANCES

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

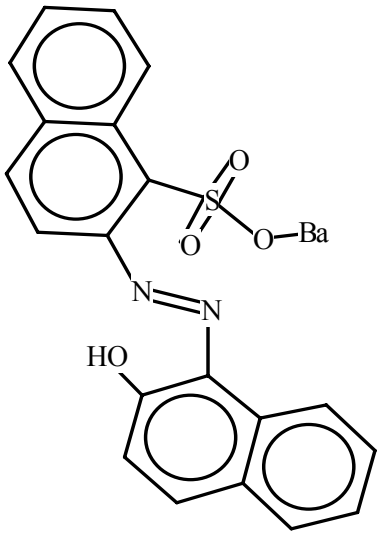
Substance name: barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate]

EC number: 214-160-6

CAS number: 1103-38-4

Molecular formula: C20H14N2O4S.1/2Ba

Structural formula:



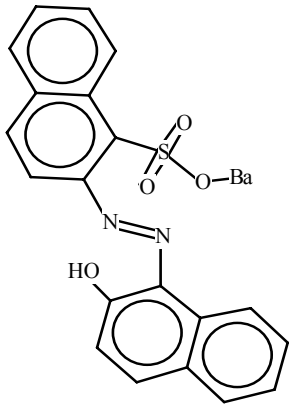
Summary of the evaluation:

Barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate] is not considered to be a PBT substance. It does not meet the B criterion. It may meet the P/vP criteria based on screening data. Ecotoxicity data was not reviewed. The assessment was partly based on data of a structurally similar substance, C.I. Pigment Red 53:1 (CAS 5160-02-1).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: Barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate]
EC Number: 214-160-6
CAS Number: 1103-38-4
IUPAC Name:
Molecular Formula: C20H14N2O4S.1/2Ba
Structural Formula:



Molecular Weight: 514.72
Synonyms: C. I. Pigment Red 49:1; C.I. No. 15630:1 (for the full list of synonyms and product names, see European Commission, 2000a)

1.1 Purity/Impurities/Additives

No data available.

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		
V, 5.3	Boiling point		
V, 5.5	Vapour pressure		
V, 5.7	Water solubility	0.00025 mg l^{-1} (at 25 ºC) 2 mg l^{-1} (room temperature) (this solubility value is for pigment red 53:1)	OECD (1999)

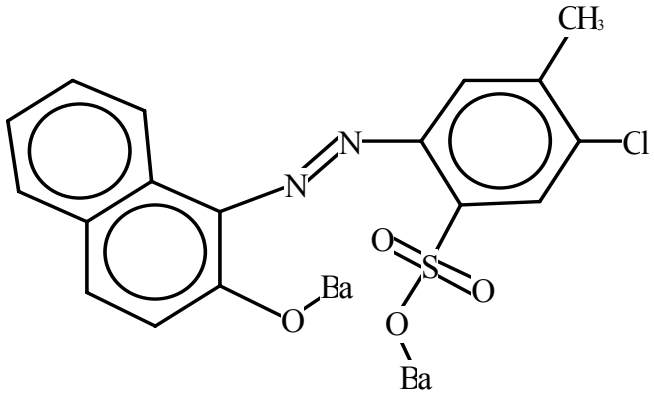
V, 5.8	Partition coefficient n-octanol/water (log value)	6.32 -0.26 -0.56	KOWWIN v1.67 (*) For Pigment Red 53:1, (measured indirectly) (*) For Pigment Red 53:1, (calculated) (*)
VII, 5.19	Dissociation constant	-5.49	For the sulphonate group based on read across from OECD (1999)(***)

(*) OECD (1999) provides a calculated logKow of –0.56 corresponding to the ionised form for a structurally similar substance C.I. Pigment Red 53:1 (CAS 5160-02-1; see Figure 1). OECD (1999) reports also a logKow of -0.26 for this substance as obtained from measured solubility in water and in octanol. KOWWIN v1.67 in turn estimates a logKow of 5.65 for the same substance. This value is (probably) calculated for the non-ionised conjugate sulphonic acid.

(**) pKa of –5.49 for the sulphonate group (for conjugate sulphonic acid) has been reported for C.I. Pigment Red 53:1 by OECD (1999). This value is due to the structural similarity applicable also to barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate] in an approximate manner. In addition, a pKa of –6.5 for aromatic sulphonic acids has been reported by Cerfontain et al. (1975)(data not evaluated).

The synonym C.I. Pigment Red 49:1 is used for the substance in this document onwards.

Figure 1 C.I. Pigment Red 53:1 (CAS 5160-02-1), a structurally similar substance



2 MANUFACTURE AND USES

Seven companies have notified the substance under Regulation 93/793/EEC. According to industry, two producers operate at the present. The substance is gained as by-product from the production of C.I. Pigment Red 53:1. The applications specified by European Commission (2000a) are uses as colouring agent and intermediate uses.

3 CLASSIFICATION AND LABELLING

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

4 ENVIRONMENTAL FATE PROPERTIES

4.1 Degradation (P)

4.1.1 Abiotic degradation

Indirect photochemical degradation in the atmosphere is considered to be fast based on the estimated half-life of 20.7 hours for the reaction with OH-radicals using AOP v1.91 (24 h day^{-1}; $5*10^5$ OH^- cm^{-3}).

No experimental data are available on abiotic degradation.

4.1.2 Biotic degradation

No experimental data are available on biodegradation. BIOWIN v4.02 predicts following biodegradation. The models provide slightly contradictory results.

Biowin 1	Biodegrades slowly (0.38)
Biowin 2	Biodegrades slowly (0.00)
Biowin 3	Months (1.8)
Biowin 4	Weeks (3.09)
Biowin 5	Biodegrades slowly (-0.70)
Biowin 6	Biodegrades slowly (0.00)
Ready biodegradability prediction:	Not readily biodegradable

The structurally similar substance pigment red 53:1 is not ready biodegradable or inherently biodegradable. 0% was degraded in 14 days in an OECD 301C test (Hoechst AG, 1993 in European Commission, 2000b) and 33% eliminated after 21 days in a Zahn-Wellens test according to DIN 38412 (reported by the same source). It must be noted, that in the inherent test, a dispersant was used and about 10% of the elimination was due to adsorption onto sludge (OECD, 1999).

4.1.3 Other information [1]

No other data are available.

4.1.4 Summary and discussion of persistence

No experimental data are available on degradation of C.I. Pigment Red 49:1. BIOWIN predicts that the substance is not readily biodegradable. The structurally similar substance C.I.Pigment Red 53:1 is persistent (not inherently biodegradable) based on the available screening biodegradation tests.

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

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

4.3 Bioaccumulation (B)

4.3.1 Screening data[2]

Based on the logKow of 6.32, BCFWIN v2.15 predicts a BCF of 65. This prediction is based on a group estimation method of limited reliability (n = 6 in the experimental database), which provides the same BCF for all ionic substances with logKow of 6 to 7.

4.3.2 Measured bioaccumulation data[3]

No experimental bioaccumulation data are available for the substance. For the structurally similar C.I. Pigment Red 53:1 (CAS 5160-02-1), a study by MITI (1992) has been reported. The test was conducted according to OECD 305 and *Cyprinus carpio* was used as test species. BCFs of 8.5-15 at test concentration of 0.07 mg l^{-1} and BCFs of 0.9-1.8 at 0.7 mg l^{-1} were measured during the 6 weeks test. It must be noted that information on the stability of the test concentration and variability of measured concentrations in fish was not provided.

4.3.3 Other supporting information[4]

No data available.

4.3.4 Summary and discussion of bioaccumulation

Based on the predicted BCF (65) and reading across from the experimental BCF (≤ 15) measured for the structurally similar substance C.I. Pigment Red 53:1 with test concentrations below water solubility, C.I. Pigment Red 49:1 is expected to have a low bioaccumulation potential.

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2 For example, log K_{ow} values, predicted BCFs

3 For example, fish bioconcentration factor

4 For example, measured concentrations in biota

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report.

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 Aquatic compartment (including sediment)

Data not reviewed for this report.

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

No data available.

6.3 Atmospheric compartment

No data available.

7 PBT AND vPvB

7.1 PBT, vPvB assessment

Persistence: C.I. Pigment Red 49:1 meets the screening P/vP criterion. The substance is not readily biodegradable based on QSAR estimations and based on read across from data of a similar substance C.I. Pigment Red 53:1 (CAS 5160-02-1). Further testing would be needed to examine the rate of degradation. Further testing is, however, not required due to the overall conclusion (see below).

Bioaccumulation: the substance does not meet the B criterion. The predicted bioconcentration factor (of limited reliability) is 56. In addition, an experimental BCF ≤ 15 was measured for the structurally similar substance C.I. Pigment Red 53:1 in a standard flow-through test with fish.

Toxicity: data not reviewed for this report.

Summary: the substance does not meet the B criterion. It may meet the P/vP criteria based on screening data. The assessment was partly based on data of the structurally similar substance C.I. Pigment Red 53:1 (CAS 5160-02-1). It is concluded that the substance 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 source:

European Commission (2000) IUCLID Dataset, barium bis[2-[(2-hydroxynaphthyl)azo]naphthalenesulphonate], CAS 1103-38-4, 18.2.2000.

Other sources:

Cerfontain H, Koeberg-Telder A and Kruk C (1975) Tetrahedron Lett., 3639 (as cited in Smith, M.B. and March, J., 2001. March's Advanced Organic Chemistry, 5th edition. John Wiley & Sons, Inc., p. 330).

European Commission (2000b) IUCLID Dataset, Barium bis[2-chloro-5-[(2-hydroxy-1-naphthyl)azo]toluene-4-sulphonate], CAS 5160-02-1, 18.2.2000.

MITI (1992) Biodegradation and Bioaccumulation data of Existing Chemicals based on CSCL Japan, Compiled under the Supervision of Chemical Products Safety Division, Basic Industries Bureau MITI, ed. by CITI, 1992. Published by Japan Chemical Industry Ecology-Toxicology & Information Center.

OECD (1999) SIDS initial assessment report, for SIAM 9, Paris, France, 29.6.-1.7.1999. Barium bis[2-chloro-5-(hydroxy-1-napthyl)azotoluene-4-sulphonate, CAS 5160-02-1. UNEP Publications.