TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

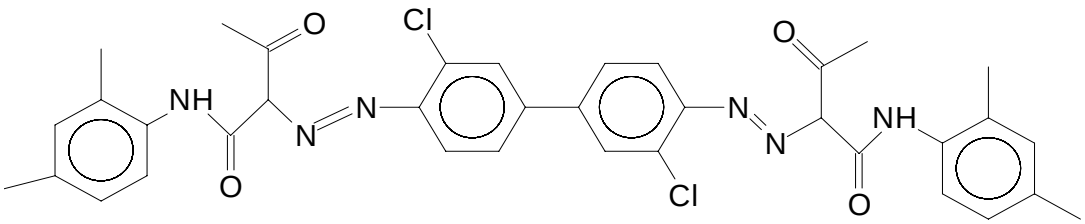
Substance name: Butanamide, 2,2'[3,3'-dichloro[1,1'-biphenyl]-4,4'diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxo- (C.I. Pigment Yellow 13)

EC number: 225-822-9

CAS number: 5102-83-0

Molecular formula: $C_{36}H_{34}Cl_2N_6O_4$

Structural formula:



Summary of the evaluation:

The substance is not considered to be a PBT or a vPvB substance. It does not meet the B (or vB) criterion, or the T criterion. It is considered likely to meet the P (and vP) criterion in order to fulfil its technical specification (it is a pigment).

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 2,2'-[3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxobutyramide]
EC Number: 225-822-9
CAS Number: 5102-83-0
IUPAC Name: Butanamide, 2,2'[3,3'-dichloro[1,1'-biphenyl]-4,4'diyl)bis(azo)]bis[N-(2,4-dimethylphenyl)-3-oxo-
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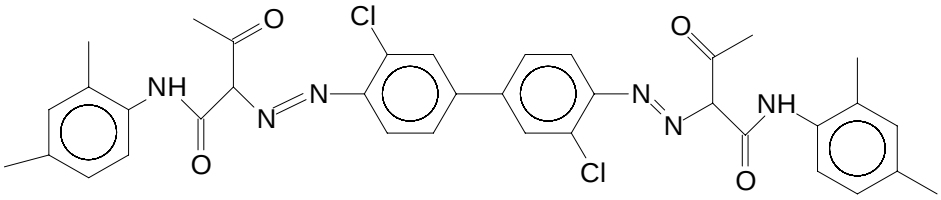

Molecular Weight: 685.62
Synonyms: C.I. 21100, Pigment Yellow 13

1.1 PURITY/IMPURITIES/ADDITIVES

Purity > 96% w/w. Typical impurities include coupling agent CAS 97-36-9 (0.5-2.5%), 3,3'-dichlorobenzidine (< 25 ppm) and water (< 1%).

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	Powder
V, 5.2	Melting / freezing point	350°C	
V, 5.3	Boiling point	N/A	
V, 5.5	Vapour pressure	6.2×10^{-21} Pa at 25°C	Calculated value at 25°C (EPIWIN v3.10)
V, 5.7	Water solubility Solubility in n-octanol	< 0.02 mg/l at 25°C < 0.02 mg/l at 25°C	Pre-treated at 80°C for 7h (as above)
V, 5.8	Partition coefficient n-octanol/water (log value)	8.1	Calculated value at 25°C
VII, 5.19	Dissociation constant		

2 MANUFACTURE AND USES

Not relevant.

3 CLASSIFICATION AND LABELLING

This substance is not classified in Annex I of Directive 67/548/EEC.

4 ENVIRONMENTAL FATE PROPERTIES

4.1 DEGRADATION (P)

4.1.1 Abiotic degradation

The calculated half-life for photo-oxidation of Pigment Yellow 13 in air is 3.1 hours. However, this substance will not be present in the air compartment due to its low volatility.

Pigment Yellow 13 is practically insoluble in water. Hydrolysis of the amide bond under environmental conditions is not likely. A half-life of >1 year was predicted using the HYDROWIN program (v1.67), but a hydrolysis study cannot be carried as the current analytical method is not sufficiently sensitive to measure the dissolved portion of this substance.

4.1.2 Biotic degradation

In a 28-day biodegradation study (COD test) performed according to OECD 301C, Pigment Yellow 13 was found to be not readily biodegradable (Madsen, 1995).

4.1.3 Other information [1]

Industry have agreed that this substance is likely to meet the P criterion in order to fulfil its technical specification (it is a pigment).

4.1.4 Summary and discussion of persistence

The results of the biodegradation test indicate that Pigment Yellow 13 is not readily biodegradable. This substance is considered to be persistent in order to perform its technical function as a pigment. Industry have agreed that it is likely to meet the P criterion.

4.2 ENVIRONMENTAL DISTRIBUTION

4.2.1 Adsorption

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

4.2.2 Volatilisation

4.3 BIOACCUMULATION (B)

4.3.1 Screening data[2]

A log K_{ow} of 8.1 (calculated at 25°C) may indicate a high potential for bioaccumulation. However, there is some uncertainty in QSAR predictions at such high log K_{ow} values. A BCF of 22,000 was calculated using equations in the TGD based on log K_{ow} of 8.1. BCF values of 10 and 9.1 were predicted using the USEPA EPIWIN BCF-program and from Banerjee et al. (1991), respectively. The difference in these values is due to the different ways the models treat substances with log K_{ow} > 6.

Other properties are considered to be relevant to the consideration of bioaccumulation for such substances (Comber et al., 2005). The solubility in octanol has been measured as 0.02 mg/l. Comber et al. (2005) propose a cut-off value for octanol solubility of 0.002 * MW mg/l, below which uptake to toxicologically significant levels is not expected. For a molecular weight of 685.62, this is a cut-off of 1.37 mg/l. The measured value is well below this, and hence indicates that Pigment Yellow 13 is not expected to accumulate to significant levels. This is supported by the lack of any indications of toxicity in exposures up to the solubility of the substance (see Section 6).

4.3.2 Measured bioaccumulation data[3]

4.3.3 Other supporting information[4]

4.3.4 Summary and discussion of bioaccumulation

Although this substance has a high predicted log K_{ow} which may indicate high bioaccumulation, other properties are considered to be more relevant for this substance. The low octanol solubility is well below the cut-off for low accumulation proposed in Comber et al. (2005). The conclusion is that the substance has a low potential for bioaccumulation.

4.4 SECONDARY POISONING

5 HUMAN HEALTH HAZARD ASSESSMENT

Data not reviewed for this report. The substance is not classified in Annex I and so has no classifications relevant to the T criterion.

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

3 For example, fish bioconcentration factor

4For example, measured concentrations in biota

6 ENVIRONMENTAL HAZARD ASSESSMENT

6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)

A chronic 21-day study with *Daphnia magna* is available for this substance (Hoechst, 1999). No adverse effects were seen at the highest concentration tested, 1 mg/l (nominal concentration). Thus the NOEC ≥ water solubility.

A study with Pigment Yellow 13 (Brown, 1981) revealed no toxicity to micro-organisms at the solubility limit. The EC_{50} was reported as >100 mg/l.

6.2 TERRESTRIAL COMPARTMENT

6.3 ATMOSPHERIC COMPARTMENT

6.4 INDIRECT EXPOSURE VIA THE FOOD CHAIN

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Pigment Yellow 13 is not readily biodegradable (OECD 301C). The substance did not degrade during the 28-day incubation period and is therefore considered to be persistent, meeting the P (and potentially the vP) criterion.

Bioaccumulation: although this substance has a high predicted log K_{ow} which might indicate a high potential for bioaccumulation, other more relevant properties indicate a low potential for bioaccumulation. In particular, the solubility in octanol is very low, 0.02 mg/l, and is well below the cut-off for significant uptake potential in Comber et al. (2005), which is calculated as 1.37 mg/l for this substance. The conclusion is therefore that the substance does not meet the B or vB criteria.

Toxicity: the 21-day NOEC for *Daphnia magna* ≥ water solubility (0.02 mg/l at 25°C). No adverse effects were seen at the highest concentration tested, 1 mg/l. Pigment Yellow 13 is not toxic towards micro-organisms at the solubility limit and based on the very low water and n-octanol solubility exposure of aquatic organisms to this substance is expected to be low. There are no relevant classifications for human health. The substance is considered not to meet the T criterion.

Summary: Pigment Yellow 13 is considered to meet the P and vP criteria with a reasonable degree of confidence. However, it does not meet the T criterion and is considered not to meet the TGD B or vB criteria. Therefore it is not considered a PBT substance according to the EU criteria.

INFORMATION ON USE AND EXPOSURE

Not relevant as substance is not identified as a PBT.

OTHER INFORMATION

The information used in this report was taken from the following source:

SIDS Initial Assessment Report for SIAM 16 (C.I. Pigment Yellow 12, 13 and 83), United Kingdom, 2003.

Discussion paper for the TC NES subgroup on PBTs, Mike Comber, Steve Robertson and Dick Sijm, 2005.