TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

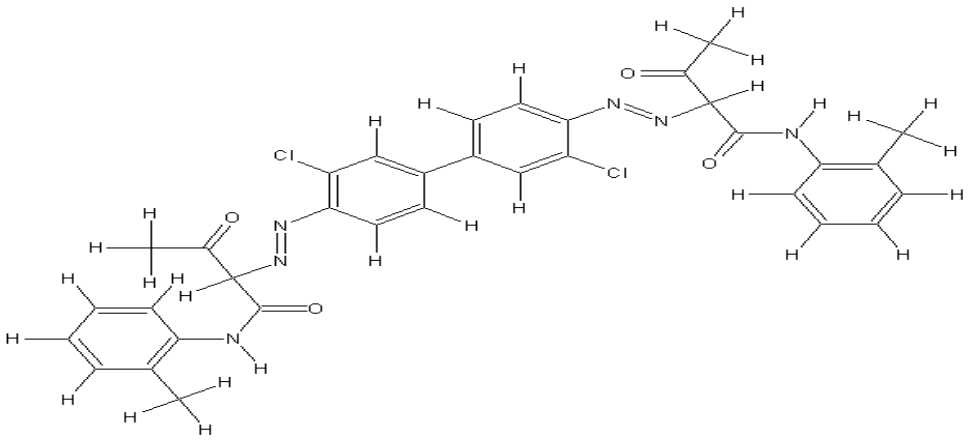
Substance name: Butanamide, 2,2'[(3,3'-dichloro[(1,1'-biphenyl)]-4,4'diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxo- (C.I. Pigment Yellow 14)

EC number: 226-789-3

CAS number: 5468-75-7

Molecular formula: $C_{34}H_{30}Cl_2N_6O_4$

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, and is considered not to meet 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-methylphenyl)-3-oxobutyramide]
EC Number: 226-789-3
CAS Number: 5468-75-7
IUPAC Name: Butanamide, 2,2'[3,3'-dichloro[1,1'-biphenyl]-4,4'diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxo-
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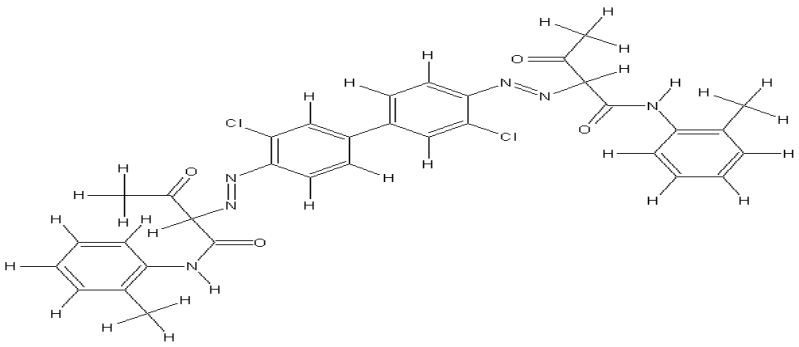

Molecular Weight: 657.56
Synonyms: C.I. 21095, Pigment Yellow 14

1.1 PURITY/IMPURITIES/ADDITIVES

No information given.

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	IUCLID (2000)
V, 5.2	Melting freezing point	349.8°C	Calculated value (EPIWIN v3.12)
V, 5.3	Boiling point	890.3°C	Calculated value (EPIWIN v3.12)
V, 5.5	Vapour pressure	2.7×10^{-22} hPa at 25°C	Calculated value at 25°C (EPIWIN v3.12)
V, 5.7	Water solubility	Not soluble 2.5×10^{-5} mg/l at 25°C	IUCLID (2000) Calculated value at 25°C using estimated log K_{ow} of 7.0 (EPIWIN v3.12)
V, 5.8	Partition coefficient n-octanol/water (log value)	7.0	Estimated value at 25°C (EPIWIN v3.12)
VII, 5.19	Dissociation constant		

2 MANUFACTURE AND USES

Not relevant.

3 CLASSIFICATION AND LABELLING

This substance is not classified in the 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 14 in air is 3.7 hours. However, this substance will not be present in the air compartment due to its low volatility.

Pigment Yellow 14 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 out as the current analytical method is not sufficiently sensitive to measure the dissolved portion of this substance.

4.1.2 Biotic degradation

No biodegradation studies are available for this substance. It is predicted to be not readily biodegradable (EPIWIN v3.12).

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

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

4.2.2 Volatilisation

4.3 BIOACCUMULATION (B)

4.3.1 Screening data[2]

A log K_{ow} of 7.0 (calculated at 25°C) may indicate a high potential for bioaccumulation. However, there is some uncertainty in QSAR predictions at high log K_{ow} values. A BCF of 10 was calculated using the USEPA EPIWIN BCF-program v2.15.

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 0.09 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 657.56, this is a cut-off of 1.32 mg/l. The measured value is well below this and hence indicates that Pigment Yellow 14 is not expected to accumulate to significant levels.

4.3.2 Measured bioaccumulation data[3]

A fish BCF test on Pigment Yellow 14 shows a BCF of < 4.9. Only a summary of the study was available. A dispersant was used and the test concentrations were indicated to be 0.1 and 1.0 mg/l

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

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

3 For example, fish bioconcentration factor

and therefore above the likely water solubility of the substance. The quality of the test was not assigned due to the lack of available information.

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 at 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.

6 ENVIRONMENTAL HAZARD ASSESSMENT

No ecotoxicological data appear to be available on Pigment Yellow 14. Based on read-across to results of fish, Daphnia and algal studies on closely related substances (Pigments Yellow 12 and 83), this substance is considered unlikely to have effects on aquatic organisms at solubility.

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Pigment Yellow 14 is predicted to be not readily biodegradable (EPIWIN v3.12). The substance is 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, 0.09 mg/l, and is well below the cut-off for significant uptake potential in Comber et al. (2005), which is calculated as 1.32 mg/l for this substance. The conclusion is therefore that the substance does not meet the B or vB criteria.

Toxicity: no ecotoxicological data appear to be available for Pigment Yellow 14. Based on read-across to results of fish, Daphnia and algal studies on closely related substances (Pigments Yellow 12 and 83), this substance is considered not to meet the T criterion.

Summary: Pigment Yellow 14 is considered to meet the P and vP criteria with a reasonable degree of confidence. However, it is considered not to meet the TGD B or vB criteria and read-across from

[4]For example, measured concentrations in biota

related substances indicates it is unlikely to meet the T criterion. 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:

IUCLID Dataset for 2,2'-[3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl)bis(azo)]bis[N-(2-methylphenyl)-3-oxobutyramide], CAS No. 5468-75-7. Non-confidential version, European Commission, 2000.

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