

TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

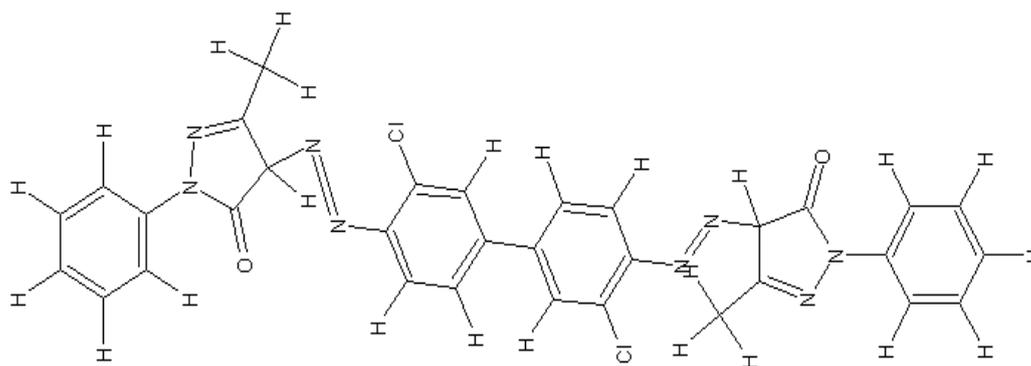
Substance name: 3H-Pyrazol-3-one, 4,4'[(3,3'-dichloro[(1,1'-biphenyl)]-4,4'-diyl)bis(azo)] bis[2,4-dihydro-5-methyl-2-phenyl- (C.I. Pigment Orange 13)

EC number: 222-530-3

CAS number: 3520-72-7

Molecular formula: C₃₂H₂₄Cl₂N₈O₂

Structural formula:



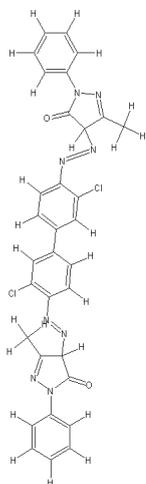
Summary of the evaluation:

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

JUSTIFICATION

1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name: 4,4'-[3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl]bis(azo)]2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-one]
EC Number: 222-530-3
CAS Number: 3520-72-7
IUPAC Name: 3H-Pyrazol-3-one, 4,4'-(3,3'-dichloro(1,1'-biphenyl)-4,4'-diyl)bis(azo)bis2,4-dihydro-5-methyl-2-phenyl-
Molecular Formula: $C_{32}H_{24}Cl_2N_8O_2$
Structural Formula:



Molecular Weight: 623.51
Synonyms: C.I. 21110, Pigment Orange 13

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	833.6°C	Calculated value (EPIWIN v3.12)
V, 5.5	Vapour pressure	1.0×10^{-20} hPa at 25°C	Calculated value at 25°C (EPIWIN v3.12)
V, 5.7	Water solubility	Not soluble 2.9×10^{-7} mg/l at 25°C	IUCLID (2000) Calculated value at 25°C using estimated log K_{ow} of 9.55 (EPIWIN v3.12)
V, 5.8	Partition coefficient n-octanol/water (log value)	9.55	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

Pigment Orange 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 out as the current analytical method is not sufficiently sensitive to measure the dissolved portion of this substance. Pigment Orange 13 will not be present in the air compartment due to its low volatility.

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 data²

A log K_{ow} of 9.55 (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. BCF values of 10 and 788 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 0.07 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 623.51, this is a cut-off of 1.25 mg/l. The measured value is well below this and hence indicates that Pigment Orange 13 is not expected to accumulate to significant levels.

4.3.2 Measured bioaccumulation data³

A fish BCF test on Pigment Orange 13 shows a BCF of 5.6. No further details of this study are available.

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

4.3.3 Other supporting information⁴

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. This 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 Orange 13. Read across from other pigments reviewed by the PBT group (Pigments Yellow 12, 14 and 83) is not considered possible due to the difference in structure.

7 PBT AND VPVB

7.1 PBT, VPVB ASSESSMENT

Persistence: Pigment Orange 13 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 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, 0.07 mg/l, and is well below the cut-off for significant uptake potential in Comber et al. (2005), which is calculated as 1.25 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 Orange 13. Due to the difference in structure to Pigments Yellow 12, 14 and 83, read-across is not considered possible.

Summary: Pigment Orange 13 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. Therefore it is not considered a PBT or a vPvB substance according to the EU criteria.

⁴For example, measured concentrations in biota

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 4,4'-[3,3'-dichloro[1,1'-biphenyl]-4,4'-diyl]bis(azo)]2,4-dihydro-5-methyl-2-phenyl-3H-pyrazol-3-one], CAS No. 3520-72-7. Non-confidential version, European Commission, 2000.

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