

## TC NES SUBGROUP ON IDENTIFICATION OF PBT AND VPVP SUBSTANCES

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

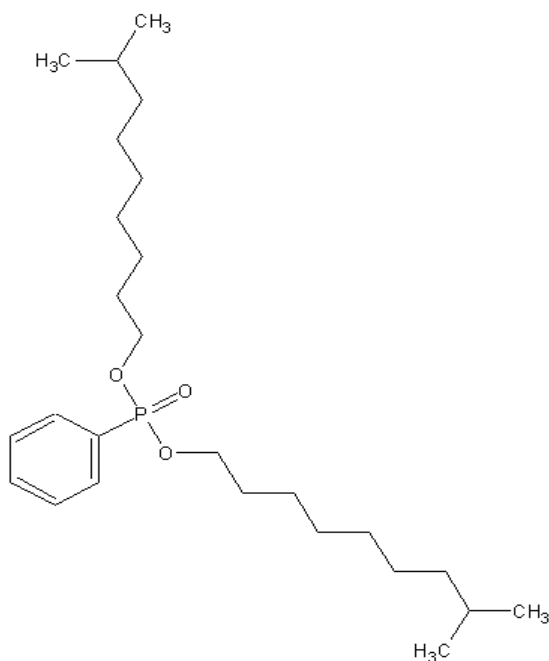
**Substance name: Diisodecyl phenyl phosphite**

**EC number: 247-098-3**

**CAS number: 25550-98-5**

**Molecular formula: C<sub>26</sub>H<sub>47</sub>O<sub>3</sub>P**

**Structural formula:**



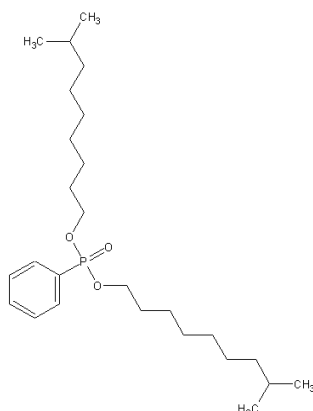
#### Summary of the evaluation:

The substance is not considered to be a PBT or a vPvB substance. It does not meet P criterion (or vP) criterion. Bioaccumulation potential is expected to be low due to hydrolysis; therefore it is not likely to meet the B (or vB) criterion.

## JUSTIFICATION

### 1 IDENTIFICATION OF THE SUBSTANCE AND PHYSICAL AND CHEMICAL PROPERTIES

Name:	Diisodecyl phenyl phosphite
EC Number:	247-098-3
CAS Number:	25550-98-5
IUPAC Name:	Phosphorous acid, diisodecyl phenyl ester
Molecular Formula:	C <sub>26</sub> H <sub>47</sub> O <sub>3</sub> P
Structural Formula:	



Molecular Weight:	438.64
Synonyms:	Irgastab CH 300; Didecylphenylphosphit; TK 11211 (IUCLID, 2000)

#### 1.1 PURITY/IMPURITIES/ADDITIVES

Purity of diisodecyl phenyl ester (CAS 25550-98-5) is 51% w/w. Impurities include:

Phosphorous acid, triphenyl ester (CAS 101-02-0) – 2% w/w;

Phosphorous acid, triisodecyl ester (CAS 25448-25-3) – 21% w/w and

Phosphorous acid, isodecyl diphenyl ester (CAS 26544-23-0) – 23% w/w.

The substance is in an equilibrium mixture of the above substances. Note, the name reflects the number of moles of isodecanol reacted with the starting triphenyl phosphite rather than describing the exact structure of what is present.

## 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	Liquid	IUCLID (2000)
V, 5.2	Melting / freezing point	90.17°C	Calculated value (EPIWIN v3.12)
V, 5.3	Boiling point	478.99°C	Calculated value (EPIWIN v3.12)
V, 5.5	Vapour pressure	2.92×10 <sup>-9</sup> hPa at 25°C	Calculated value at 25°C (EPIWIN v3.12)
V, 5.7	Water solubility - Diisodecyl phenyl phosphite	1.91×10 <sup>-5</sup> mg/l at 25°C 2.1×10 <sup>-4</sup> mg/l	Calculated value at 25°C using estimated log K <sub>ow</sub> of 9.32 (EPIWIN v3.12) Estimated from fragments (EPIWIN v3.12)
	Water solubility - Triphenyl phosphite	0.3 mg/l at 25°C (not possible to measure value due to hydrolysis during the test)	Calculated value (Reimer Analytical & Associates Inc., 2002)
V, 5.8	Partition coefficient n-octanol/water (log value)	9.32	Estimated value (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

An OECD 111 test (modified due to the poor solubility of the material) performed on diisodecyl phenyl phosphite showed rapid hydrolysis within 24 hours at pH 4, 7 and 10. Appreciable hydrolysis occurred up to 24 hours, but further hydrolysis seemed to be hindered perhaps due to micelle formation. Up to 72% hydrolysis was observed at pH 4 after 24 hours (hydrolysis is faster in acid than base).

An experiment was carried out to measure the hydrolysis rates of a related substance, triphenyl phosphite, in unstirred buffer solutions containing 50% CH<sub>3</sub>CN cosolvent. The observed half-lives were 46, 16 and 1 d at pH 5, 7 and 9, respectively. It was concluded that the half-lives of triphenyl phosphite under the OECD hydrolysis test conditions are likely to be < 1 year (OECD threshold half-life) and triphenyl phosphite would be classed as a hydrolytically unstable compound.

There are some indications of the disappearance of the substance from water in ecotoxicity tests (see Section 6.1.1).

#### **4.1.2 Biotic degradation**

No significant biodegradation (10% after 28 days) was observed in a modified Sturm test (IUCLID, 2000). However, the water solubility of diisodecyl phenyl phosphite predicted using EPIWIN v3.12 is very low (< 0.001 mg/l). Therefore the low level of degradation observed may be misleading as very little of the added substance (the test was performed at a concentration of 10.9 mg/l.) would be available in solution.

#### **4.1.3 Other information <sup>1</sup>**

#### **4.1.4 Summary and discussion of persistence**

Phosphorous-oxygen-carbon bonds of phosphites readily hydrolyse in water to yield phosphorous acid and the corresponding alcohol or phenol. Diisodecyl phenyl phosphite shows rapid hydrolysis within 24 hours at pH 4, 7 and 10. Thus hydrolysis will be a key feature in the fate of this substance, particularly at concentrations close to the water solubility limit. Furthermore, it is likely that related substance triphenyl phosphite would be classified as a hydrolytically unstable compound based on the results of a modified hydrolytic stability experiment.

The low level of biodegradation observed in a modified Sturm test (IUCLID, 2000) may be misleading since the test used a concentration much higher than the expected water solubility of the test substance and so very little of the added substance would be available in solution for biodegradation.

### **4.2 ENVIRONMENTAL DISTRIBUTION**

#### **4.2.1 Adsorption**

#### **4.2.2 Volatilisation**

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<sup>1</sup> For example, half life from field studies or monitoring data

### **4.3 BIOACCUMULATION (B)**

#### **4.3.1 Screening data<sup>2</sup>**

A log  $K_{ow}$  of 9.32 (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 value of 3.16 was predicted using EPIWIN (v2.15).

#### **4.3.2 Measured bioaccumulation data<sup>3</sup>**

None available.

#### **4.3.3 Other supporting information<sup>4</sup>**

#### **4.3.4 Summary and discussion of bioaccumulation**

This substance has a high predicted log  $K_{ow}$  which may indicate high bioaccumulation. However, due to rapid hydrolysis of this substance, an actual measurement of  $K_{ow}$  may be difficult and a BCF test not possible. Furthermore, the utility of a partition coefficient in determining the bioaccumulation potential of hydrolytically unstable substance is questionable. The hydrolysis products of this substance (phosphorous acid, isodecanol and phenol) are not considered bioaccumulative.

### **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**

### **6.1 AQUATIC COMPARTMENT (INCLUDING SEDIMENT)**

Acute aquatic toxicity data are available for fish, Daphnia and algae (IUCLID, 2000). Tests used concentrations much higher than the expected water solubility of the substance. Daphnia appeared to be the most sensitive species (48-hour  $EC_{50} = 0.2$  mg/l), but it is possible that this might have been due to physical effects or to the soluble fraction of the substance and/or hydrolysis products. Rapid disappearance of the test substance (> 50-100%) in the fish and Daphnia toxicity tests has

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<sup>2</sup> For example, log  $K_{ow}$  values, predicted BCFs

<sup>3</sup> For example, fish bioconcentration factor

<sup>4</sup> For example, measured concentrations in biota

been reported by Industry, although the current IUCLID entry states that analytical monitoring was not carried out for the fish test.

## **7 PBT AND VPVB**

### **7.1 PBT, VPVB ASSESSMENT**

**Persistence:** Diisodecyl phenyl phosphite shows rapid hydrolysis within 24 hours at pH 4, 7 and 10. Hydrolysis is a key feature in the fate of this substance. The low level of biodegradation observed in a modified Sturm test may be misleading since the test used a concentration much higher than the expected water solubility of the test substance and so most of the added substance would not be available for biodegradation. The related substance triphenyl phosphite is likely to be classified as a hydrolytically unstable compound. In conclusion, diisodecyl phenyl phosphite is considered not to be persistent and the P (and vP) criterion is not met.

**Bioaccumulation:** this substance has a high predicted log  $K_{ow}$  which may indicate high bioaccumulation. However, the bioaccumulation potential is expected to be low due to rapid hydrolysis in the environment. The hydrolysis products (phosphorous acid, isodecanol and phenol) are not considered to be accumulative. The substance is considered not to meet the B criterion.

**Toxicity:** all tests used concentrations much higher than the expected water solubility of the test substance, thus the available acute toxicity data may not be valid. Also, diisodecyl phenyl phosphite undergoes rapid hydrolysis in water. On the basis of the reported data, the screening T criterion is not met, although if the effects reported are genuine and due to the dissolved substance, then the criterion might be met.

**Summary:** the substance does not meet the P or vP criteria. Bioaccumulation potential is expected to be low due to hydrolysis, therefore it is considered not to meet the B or vB criteria. Diisodecyl phenyl phosphite is not considered a PBT or a vPvB 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 Diisodecyl Phenyl Phosphite, CAS No. 25550-98-5. Non-confidential version, European Commission, 2000.

Physical/Chemical Property of Triphenyl Phosphite (TPPi), CAS No. 101-02-0: Water Solubility (OECD 105) and Hydrolytic Stability (OECD 111). Reimer Analytical & Associates Inc., 2002.