

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

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

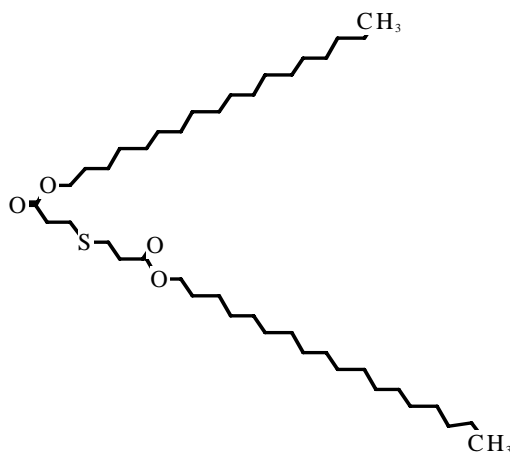
**Substance name:** Dioctadecyl 3,3'-thiodipropionate

**EC number:** 211-750-5

**CAS number:** 693-36-7

**Molecular formula:** C<sub>42</sub>H<sub>82</sub>O<sub>4</sub>S

**Structural formula:**



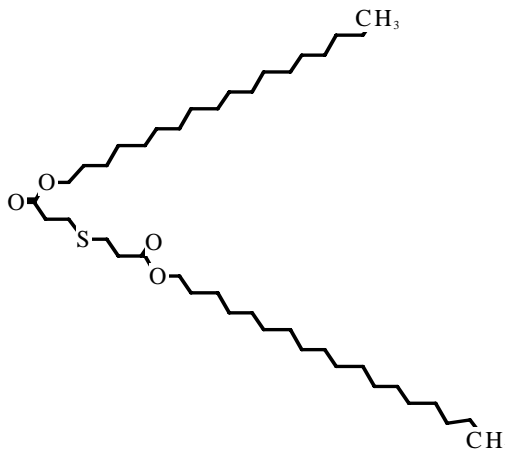
#### Summary of the evaluation:

Dioctadecyl 3,3'-thiodipropionate is not considered as a PBT –substance. It does not meet the P/vP –criteria based on screening data. Assessments of bioaccumulation and ecotoxicity were not finalized/carried out.

## JUSTIFICATION

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

Name: Dioctadecyl 3,3'-thiodipropionate  
EC Number: 211-750-5  
CAS Number: 693-36-7  
IUPAC Name:  
Molecular Formula: C<sub>42</sub>H<sub>82</sub>O<sub>4</sub>S  
Structural Formula:



Molecular Weight: 683.18  
Synonyms: Dioctadecyl 3,3'-thiodipropionate  
Dioctadecyl thiodipropionate  
Distearyl.beta.-beta.'-thiodipropionate  
Distearyl.beta.-thiodipropionate  
Distearyl 3,3'-thiodipropionate  
Distearyl thiodipropionate  
Propanoic acid, 3,3'-thibis-, dioctadecyl ester (9CI)  
Propanoic acid, 3,3'-thidi-, dioctadecyl ester (6CI, 8CI)  
Stearyl 3,3'-thiodipropionate

#### 1.1 Purity/Impurities/Additives

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#### 1.2 Physico-Chemical properties

Table 1 Summary of physico-chemical properties. For details and references, see European Commission (2000). It is noted, that the data were not evaluated by the Rapporteur.

REACH ref Annex, §	Property	Value	Comments
VII, 7.1	Physical state at 20 °C and 101.3 Kpa	solid	European Commission 2000
VII, 7.2	Melting / freezing point	64-67 °C	Ciba Additive GmbH, 1991
VII, 7.3	Boiling point	-	
VII, 7.5	Vapour pressure	0.0000066 hPa at 20 °C	Ciba Additive GmbH, 1985
VII, 7.7	Water solubility	3.617×10 <sup>-14</sup> mg/l at 25 °C <0.001 g/l at 20 °C	Estimate from Log Kow (WSKOW v1.41) Ciba Additive GmbH
VII, 7.8	Partition coefficient n-octanol/water (log value)	17.68 >6 at 20 °C	Estimate (KOWWIN v1.67) Calculated, Ciba Additive GmbH
	Dissociation constant	-	

## 2 MANUFACTURE AND USES

Four producers/importers have provided data under Regulation 93/793/EEC. The substance is according to European Commission (2000) produced/imported in quantities between 5,000 – 10,000 tonnes per year and used as a stabilizer and antioxidant.

## 3 CLASSIFICATION AND LABELLING

The substance is not classified under 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 5.6 hours for the reaction with OH-radicals using AOP v1.91 (24 h day<sup>-1</sup>; 5\*10<sup>5</sup> OH<sup>-</sup> cm<sup>-3</sup>).

#### 4.1.2 Biotic degradation

An OECD 301 B (modified Sturm test) resulted in a mineralization of 2 % in 28 days using a test concentration of 23.9 mg/l and activated sludge as an inoculum (Ciba Additive GmbH). Another available record on an OECD 301 B –test reports a mineralization of 15 % in 28 days. In this test a test concentration of 11.3 mg/l and activated sludge were employed (Ciba Additive GmbH). It is noted, that the study report was not available to the Rapporteur for evaluation.

The degradability of dioctadecyl 3,3'-thiodipropionate (DSTDP) was studied by Akzo Nobel (2006) in a closed bottle test according to OECD 301 D with slight modifications. Test substance dissolved in dichloromethane was added to 250-300 ml BOD bottles. Thereafter, the dichloromethane was

evaporated during 24 hours on a roller bank before adding mineral medium and inoculum. The DSTDP concentration was 2 mg/l and the concentration of inoculum (secondary activated sludge derived from a municipal STP) was 2 mg dw/l. The test bottles were placed on magnetic stirrers and were incubated in the dark at 19-21 °C for 28 days. Two duplicate bottles were withdrawn for analyses of dissolved oxygen at days 7, 14, 21 and 28. The biodegradation of DSTDP was 71% in 28 days based on the BOD/ThOD-ratio (see Table 4.1). To conclude, DSTDP is on the border of meeting the criteria for ready biodegradability. It reaches the pass level of 60% biodegradation in 21 days but fails to meet the 10-day window criterion.

Table 4.1. Biodegradation of DSTDP in a closed bottle test of Akzo Nobel (2006).

Time	Oxygen consumption (mg/l)	Biodegradation (%; BOD/ThoD)
0	0	0
7	1.4	24
14	2.7	47
21	3.5	60
28	4.1	71

BIOWIN v4.02 provides following predictions: BIOWIN2 = 0.99, BIOWIN3 = 2.57 and BIOWIN6 = 0.98.

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

No data available.

#### 4.1.4 Summary and discussion of persistence

Due to the very low solubility and high adsorption potential, the modified OECD 301 D test result (71 % in 28 days) is considered to reflect more appropriately the biodegradation potential of the substance than the results of two OECD 301 B –tests (2 % in 28 days and 15 % in 28 days). Based on the modified OECD 301 D test result, the substance is considered as readily biodegradable without meeting the 10-day window. The BIOWIN predictions support this result. The substance is concluded to be not persistent.

#### 4.2 Environmental distribution

Data not reviewed for this report.

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

**4.2.1 Adsorption****4.2.2 Volatilisation****4.2.3 Long-range environmental transport****4.3 Bioaccumulation (B)****4.3.1 Screening data**

An estimated logKow of 17.68 is available for the substance. BCFWIN vv2.15 provides a BCF of 3.2.

**4.3.2 Measured bioaccumulation data**

No experimental data are available on the substance.

**4.3.3 Other supporting information<sup>2</sup>**

No data available.

**4.3.4 Summary and discussion of bioaccumulation**

No experimental data on bioaccumulation are available for the substance. A logKow of 17.68 indicates limited bioconcentration. However, further information is necessary to complete the assessment of bioaccumulation.

**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.

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<sup>2</sup>For example, measured concentrations in biota

## **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**

No data available.

## **6.1.3 Other aquatic organisms**

Data not evaluated for this report.

## **6.2 Terrestrial compartment**

No data available.

## **6.3 Atmospheric compartment**

No data available.

## **7 PBT AND vPvB**

### **7.1 PBT, vPvB assessment**

Persistence: Dioctadecyl 3,3'-thiodipropionate is considered to not meet the P/vP -criteria according to screening data. 71 % of the substance degraded in a modified OECD 301 D (closed bottle) –test in 28 days. The QSAR-predictions support the result.

**Bioaccumulation:** The assessment of bioaccumulation was not finalised. An estimated logKow of 17.68 indicate limited bioconcentration, but further information is needed to complete the assessment.

**Toxicity:** No assessment of ecotoxicity was carried out.

**Summary:** Dioctadecyl 3,3'-thiodipropionate does not meet the P/vP –criteria based on screening data. Assessments of bioaccumulation and ecotoxicity were not finalized/carried out. The substance is concluded not to be 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, Dioctadecyl 3,3'-thiodipropionate, CAS 693-36-7, 19.2.2000.

Other sources:

Akzo Nobel (2006). Dioctadecyl 3,3'-thiodipropionate, Ready Biodegradability Closed Bottle Test. Report No: CER F06010, April 25, 2006.