

## SORBITAN, MONODODECANOATE, POLY (OXY-1,2-DIETHANEDIYL)

This dossier on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) presents the most critical studies pertinent to the risk assessment of sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) in its use in drilling muds. This dossier does not represent an exhaustive or critical review of all available data. The information presented in this dossier was obtained primarily from the ECHA database that provides information on chemicals that have been registered under the EU REACH (ECHA). Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch et al., 1997).

Screening Assessment Conclusion – Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is classified as a **tier 1** chemical and requires a hazard assessment only.

### 1 BACKGROUND

Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is a hydrophilic, non-ionic surfactant used as an emulsifier. It is considered a UVCB substance (substance of unknown or variable composition, complex reaction products or biological materials). Based on the substance group types evaluated, the substance is readily biodegradable; has a low potential for bioaccumulation; and a high potential for adsorption to soil and sediment. It is of low-to-moderate toxicity concern to aquatic life.

### 2 CHEMICAL NAME AND IDENTIFICATION

**Chemical Name (IUPAC):** Sorbitan monolaurate, ethoxylated

**CAS RN:** 9005-64-5

**Molecular formula:** Not available (UVCB substance)

**Molecular weight:** Not available (UVCB substance)

**Synonyms:** See below.

The composition of sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) (CAS No. 9005-64-5) is unknown. The CAS No. 9005-64-5 is a generic CAS No. that can include at least the following UVCB substance groups:

1. A mixture of laurate esters of sorbitol and sorbitol anhydrides, consisting predominantly of the monoester, condensed with approximately 4 moles of ethylene oxide (e.g., Polysorbate 21).
2. An ethoxylated sorbitan ester of lauric acid with an average of 10 moles of ethylene oxide (e.g., PEG-10 sorbitan laurate).
3. A mixture of laurate esters of sorbitol and sorbitol anhydrides, consisting predominantly of the monoester, condensed with approximately 20 moles of ethylene oxide (e.g., Polysorbate 20).

4. An ethoxylated sorbitan ester of lauric acid with an average of 40 moles of ethylene oxide (e.g., PEG-40 sorbitan laurate).

5. An ethoxylated sorbitan ester of lauric acid with an average of 44 moles of ethylene oxide (e.g., PEG-44 sorbitan laurate).

6. An ethoxylated sorbitan ester of lauric acid with an average of 75 moles of ethylene oxide (e.g., PEG-75 sorbitan laurate).

7. An ethoxylated sorbitan ester of lauric acid with an average of 80 moles of ethylene oxide (e.g., PEG-80 sorbitan laurate).

This dossier will include information from the following substances:

Polysorbate 20 (CAS No. 9005-64-5)

Sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5]

### 3 PHYSICO-CHEMICAL PROPERTIES

Key physical and chemical properties for the substance are shown in Table 1.

**Table 1 Overview of the Physico-chemical Properties of Sorbitan Monolaurate, Ethoxylated (1 - 6.5 Moles Ethoxylated) (CAS No. 9005-64-5)**

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Lemon- to amber-coloured oily liquid	2	ECHA
Melting point	-64 to -22°C @ 101.3 kPa	2	ECHA
Boiling point	-	-	-
Density	1095 kg/m <sup>3</sup> @ 20°C	2	ECHA
Vapour pressure	Negligible	2	ECHA
Partition coefficient (log K <sub>ow</sub> )	1.23 to 3.86 (QSAR)	2	ECHA
Water solubility	<0.0002 g/L @ 20°C	1	ECHA
Dissociation constant (pK <sub>a</sub> )	13.84 – 13.89 @ 20°C	2	ECHA

### 4 DOMESTIC AND INTERNATIONAL REGULATORY INFORMATION

A review of international and national environmental regulatory information was undertaken (Table 2). This chemical is listed on the Australian Inventory of Chemical Substances – AICS (Inventory). No conditions for its use were identified. No specific environmental regulatory controls or concerns

were identified within Australia and internationally for sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl).

**Table 2 Existing International Controls**

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No
Rotterdam Convention	No
Stockholm Convention	No
REACH (Substances of Very High Concern)	No
United States Endocrine Disrupter Screening Program	No
European Commission Endocrine Disruptors Strategy	No

## 5 ENVIRONMENTAL FATE SUMMARY

### A. Summary

Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is readily biodegradable; has a low potential for bioaccumulation; and a high potential for adsorption to soil and sediment.

### B. Biodegradation

In an OECD 301F study, there was 62.5% degradation after 28 days (ECHA) [Kl. score = 1]. The results indicate that this substance is readily biodegradable even though it did not meet the 10-day window because the criterion does not apply to multi-component substance when assessing their ready biodegradability (ECHA) [Kl. score = 1]. If a chemical is found to be readily biodegradable, it is categorised as Not Persistent since its half-life is substantially less than 60 days (DoEE, 2017).

### C. Environmental Distribution

No experimental studies are available on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl). Using KOCWIN v2.00,  $K_{oc}$  values were calculated for the following constituents (ECHA) [Kl. score = 2]:

C12 fatty acid EO1:  $K_{oc}$  = 53.81

C12 fatty acid EO7:  $K_{oc}$  = 116

The  $K_{oc}$  values indicate a low adsorption potential and high potential for mobility. However, these substances also have a potential for surface active properties, which is not accounted for in the QSAR model calculations. The adsorption of non-ionic surfactants to soil is generally high as shown in experimental studies on Polysorbate 80 (CAS No. 9005-65-6) (ECHA). Consequently, sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is expected to adsorb to soil or sediments similar to other sorbitan esters.

#### D. Bioaccumulation

No experimental studies are available on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl). The bioconcentration factor (BCF) was estimated using the QSAR model BCFBAF v3.01 (ECHA). Using the Arnot-Gobas method, BCF values of 1.2 to 7.1 were calculated for the main constituents. When biotransformation was excluded, the BCF values of 2.7 to 758 L/kg were obtained. These results indicated that there is extensive metabolism of Polysorbate 20, and thus the bioaccumulation potential of Polysorbate 20 is low (ECHA) [Kl. score = 2].

### 6 ENVIRONMENTAL EFFECTS SUMMARY

#### A. Summary

Polysorbate 20 is of low-to-moderate toxicity concern to aquatic life. Data to support this conclusion are discussed below.

#### B. Aquatic Toxicity

##### Acute Studies

Table 3 lists the results of acute aquatic toxicity studies conducted on sorbitan monolaurate, ethoxylated (1 – 6.5 moles ethoxylated).

**Table 3 Acute Aquatic Toxicity Studies on Sorbitan Monolaurate, Ethoxylated (1-6.5 Moles Ethoxylated) [CAS No. 9005-64-5]**

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Brachydanio rerio</i>	96-hr LL <sub>50</sub>	>100 [WAF]	2	ECHA
<i>Pseudokirchneriella subcapitata</i>	72-hr EL <sub>50</sub>	58.84 [WAF]	2	ECHA

##### Chronic Studies

The 21-day NOELR (no-observed-effect-loading-rate) for sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5] in a *Daphnia* reproduction test was 10 mg/L WAF (ECHA) [Kl. score = 2].

The 72-hr EL<sub>10</sub> for sorbitan monolaurate, ethoxylated (1-6.5 moles ethoxylated) [CAS No. 9005-64-5] to *Pseudokirchneriella subcapitata* is 19.05 mg/L WAF (ECHA) [Kl. score = 2].

#### C. Terrestrial Toxicity

No studies are available.

## **7 CATEGORISATION AND OTHER CHARACTERISTICS OF CONCERN**

### **A. PBT Categorisation**

The methodology for the Persistent, Bioaccumulative and Toxic (PBT) substances assessment is based on the Australian and EU REACH Criteria methodology (DEWHA, 2009; ECHA, 2008).

Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is readily biodegradable; thus, it does not meet the screening criteria for persistence.

Based on calculate BCF values of 1.2 to 7.1, sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is >0.1 mg/L WAF. The acute EL<sub>50</sub> values for sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) in fish and algae are >1 mg/L WAF. Thus, sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) does not meet the criteria for toxicity.

The overall conclusion is that sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl) is not a PBT substance.

### **B. Other Characteristics of Concern**

No other characteristics of concern were identified for sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl).

## 8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment <sup>1</sup>	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required <sup>3</sup>
			Listed as a COC on relevant databases?	Identified as Polymer of Low Concern	P criteria fulfilled?	Other P Concerns	B criteria fulfilled?	T criteria fulfilled?	Acute Toxicity <sup>2</sup>	Chronic Toxicity <sup>2</sup>	
Sorbitan, monododecanoate, poly (oxy-1,2-diethandiyl)	9005-64-5	Not a PBT	No	No	No	No	No	No	1	1	1

**Footnotes:**

1 – PBT Assessment based on PBT Framework.

2 – Acute and chronic aquatic toxicity evaluated consistent with assessment criteria (see Framework).

3 – Tier 1 – Hazard Assessment only.

**Notes:**

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

## 9 REFERENCES, ABBREVIATIONS AND ACRONYMS

### A. References

Department of the Environment, Water, Heritage and the Arts [DEWHA] (2009). Environmental risk assessment guidance manual for industrial chemicals, Department of the Environment, Water, Heritage and the Arts, Commonwealth of Australia.

Department of the Environment and Energy [DoEE]. (2017). Chemical Risk Assessment Guidance Manual: for chemicals associated with coal seam gas extraction, Guidance manual prepared by Hydrobiology and ToxConsult Pty Ltd for the Department of the Environment and Energy, Commonwealth of Australia, Canberra.

ECHA. ECHA REACH database: <http://echa.europa.eu/information-on-chemicals/registered-substances>

European Chemicals Agency [ECHA] (2008). Guidance on Information Requirements and Chemical Safety Assessment, Chapter R11: PBT Assessment, European Chemicals Agency, Helsinki, Finland.

Klimisch, H.J., Andreae, M., and Tillmann, U. (1997). A systematic approach for evaluating the quality of experimental and toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

### B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
BCF	Bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
ECHA	European Chemicals Agency
EL	Effective level
EU	European Union
g/L	grams per litre
IUPAC	International Union of Pure and Applied Chemistry
kg/m <sup>3</sup>	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram

LL	Lethal level
mg/L	milligrams per litre
NOELR	no-observed-effect-loading-rate
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials