

SODIUM LAURYL POLYOXYETHYLENE ETHER SULFATE

This dossier on sodium lauryl polyoxyethylene ether sulfate presents the most critical studies pertinent to the risk assessment of this chemical in its use in coal seam gas extraction activities. This dossier does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained 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 – Limited information is available for sodium lauryl polyoxyethylene ether sulfate, and as a result sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES) has been selected as a surrogate chemical for this review. Based on this read-across data, sodium lauryl polyoxyethylene ether sulfate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium lauryl polyoxyethylene ether sulfate is an anionic surfactant detergent. The chemicals in this group are structurally related salts of sulfated ethoxylated lauryl alcohol. Sodium lauryl polyoxyethylene ether sulfate (also known as sodium laureth sulfate), CAS No. 9004-82-4, is a generic CAS registration number that includes the group of chemicals with CAS Nos 15826-16-1, 3088-31-1, 13150-00-0, and 66161-57-7, where they have an average of one, two, three, and 12 ethoxylate units, respectively. Chemical-specific information from group member sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES) (CAS No. 3088-31-1) was used for this review. SDES is readily biodegradable. It has a strong potential for sorption to soil and sediment. However, it is not expected to bioaccumulate. SDES is of low acute and chronic toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): sodium;2-dodecoxyethyl sulfate

CAS RN: 9004-82-4

Molecular formula: C₁₄H₂₉NaO₅S

Molecular weight: 332.43 g/mol

Synonyms: sodium lauryl polyoxyethylene ether sulfate; sodium laureth sulfate; dodecyl sodium ethoxysulfate

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 Sodium 2-(2-Dodecyloxyethoxy) Ethyl Sulfate¹

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Odourless and colourless liquid	1	ECHA
Melting Point	Not available	-	-
Boiling Point	113.4 °C @92 kPa	1	ECHA
Density	1990 kg/m ³ @ 20°C	1	ECHA
Vapour Pressure	1.33 x 10 ⁻¹⁰ Pa @ 25°C	1	ECHA
Partition Coefficient (log K _{ow})	-0.602 @ 39°C	1	ECHA
Water Solubility	1000 g/L @ 39°C	1	ECHA
Dissociation Constant (pKa)	2.2 x 10 ⁻¹⁸ @ 20°C	1	ECHA

¹ - Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data is shown for read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (CAS No. 3088-31-1).

The chemicals in this group are structurally related salts of sulfated ethoxylated lauryl alcohol. The synthesis of the chemicals occurs through similar processes. Lauryl alcohol is ethoxylated with ethylene oxide to form a polyethoxy ether. The terminal alcohol group is then sulfated with sulfur trioxide. The product is neutralised with either sodium or ammonium hydroxide, producing the chemicals of this group. The sodium and ammonium ions are not expected to significantly affect the hazardous properties of the chemicals.

The number of ethoxylate units usually has an average value between one and four. Sodium laureth sulfate, CAS No. 9004-82-4, is a generic CAS registration number that includes the group of chemicals with CAS Nos 15826-16-1, 3088-31-1, 13150-00-0, and 66161-57-7, where they have an average of one, two, three, and 12 ethoxylate units, respectively.

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 sodium lauryl polyoxyethylene ether sulfate.

Table 2 Existing International Controls

Convention, Protocol or other international control	Listed Yes or No?
Montreal Protocol	No
Synthetic Greenhouse Gases (SGG)	No

Convention, Protocol or other international control	Listed Yes or 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

Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data is shown for read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES, CAS No. 3088-31-1).

SDES is readily biodegradable. It has a strong potential for sorption to soil and sediment. However, it is not expected to bioaccumulate.

B. Partitioning

SDES is highly soluble in water. Volatilization from water or moist soil surfaces is not expected to be an important fate process based upon its water solubility and that it is an ionic compound. It is not expected to volatilize from dry soil surfaces based upon its estimated vapour pressure.

The hydrolysis rate constant of sodium 2-(2-dodecyloxyethoxy) ethyl sulfate is estimated to be 454767×10^{-11} cm³/molecule-sec. at half life of 2.822 hrs. The estimated half life of the substance indicates that the substance is moderately hydrolysable (ECHA) [KI. Score = 2].

C. Biodegradation

By applying weight of evidence approach, SDES was found to be readily biodegradable with 50% to 71.199 % percentage degradation (ECHA) [KI. Score = 2]. 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).

D. Environmental Distribution

No experimental data are available for SDES. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value from the molecular connectivity index (MCI) and log K_{oc} are 2,111 and 3.324 L/kg, respectively (ECHA). Based on this K_{oc} value, if released to soil, SDES is expected to strongly adsorb to soil and have a low potential for mobility. If released to water, based on the K_{oc} value and its high water solubility, it is also expected to adsorb to suspended solids and sediment.

E. Bioaccumulation

There are no bioaccumulation studies on SDES. The BCF was estimated to vary between 70.79 and 72.127 in aquatic organisms and fish (ECHA) [KI. Score = 2]. Based on the log K_{ow} (-2.03) and the calculated BCFs, bioaccumulation is not to be expected.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data is shown for read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (SDES, CAS No. 3088-31-1).

SDES is of low acute and chronic toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on SDES.

Table 3 Acute Aquatic Toxicity Studies on SDES (CAS No. 3088-31-1)

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Danio rerio</i>	96-hour LC ₅₀	25	2	ECHA
<i>Danio rerio</i>	96-hour LC ₅₀	102.59	2	ECHA
<i>Oryzias latipes</i>	48-hour LC ₅₀	46	2	ECHA
<i>Daphnia magna</i>	48-hour LC ₅₀	86.09	2	ECHA
<i>Pseudokirchneriella subcapitata</i>	72-hour EC ₅₀ (growth rate)	115.072	2	ECHA
<i>Laminaria hyperborea</i>	24-hour EC ₅₀	100 (cell changes)*	2	ECHA

*Data for CAS No. 9004-82-4 (SLES).

Chronic Studies

Based on the prediction done using ECOSAR version 1.1, the long term toxicity on fish was predicted for SDES. On the basis of effects observed in a static fresh water system, the NOEC value for the substance is estimated to be 36.507 mg/L for fish for 28 days of exposure duration (ECHA) [Kl. Score = 2].

Based on the prediction done using ECOSAR version 1.1, the long term toxicity on aquatic invertebrate was predicted for SDES. On the basis of effects observed in a static freshwater system, the NOEC value for the test substance is estimated to be 20.059 mg/L for aquatic invertebrate for 21 days of exposure (ECHA) [Kl. Score = 2].

Since SDES is readily biodegradable in an aquatic environment it can be concluded that the test chemical can be considered as non-toxic to fish and aquatic invertebrates at environmentally relevant concentrations (ECHA).

C. Terrestrial Toxicity

The lethal concentration (LC50) of SDES in soil macroorganism [*Eisenia fetida* (worms)] in a long term toxicity study of 14 days on the basis of mortality effect was estimated to be 2600 mg/kg soil dw (ECHA) [Kl. Score = 2].

The effective concentration (EC50) of SDES in terrestrial plants (*Lactuca sativa*) in short term toxicity study of 72 hrs. on the basis of reproduction effect was estimated to be 143.2 mg/kg soil dw (ECHA) [Kl. Score = 2].

Considering that the chemical is readily biodegradable in soil, it is expected that the chemical SDES shall not exhibit toxicity to soil microorganism, terrestrial plants, terrestrial arthropods and soil microorganisms (ECHA).

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).

Sodium lauryl polyoxyethylene ether sulfate is readily biodegradable; thus, it does not meet the screening criteria for persistence.

No data are available on bioaccumulation. However, based on the low log K_{ow} and calculated BCFs, bioaccumulation is not expected. Thus, sodium lauryl polyoxyethylene ether sulfate does not meet the screening criteria for bioaccumulation.

The NOECs from the chronic aquatic toxicity studies on sodium lauryl polyoxyethylene ether sulfate are >0.1 mg/L. The EC₅₀ values for sodium lauryl polyoxyethylene ether sulfate are > 1 mg/L. Thus sodium lauryl polyoxyethylene ether sulfate, does not meet the criteria for toxicity.

Therefore, SDS is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium lauryl polyoxyethylene ether sulfate.

8 SCREENING ASSESSMENT

Chemical Name	CAS No.	Overall PBT Assessment ¹	Chemical Databases of Concern Assessment Step		Persistence Assessment Step		Bioaccumulative Assessment Step	Toxicity Assessment Step			Risk Assessment Actions Required ³
			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 ²	Chronic Toxicity ²	
Sodium lauryl polyoxyethylene ether	9004-82-4	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). Chemical-specific data is not available for sodium lauryl polyoxyethylene ether sulfate. Data from read-across chemical sodium 2-(2-dodecyloxyethoxy) ethyl sulfate (CAS No. 3088-31-1) was used.

3 - Tier 1 - Hazard Assessment only.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

9 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
AICS	Australian Inventory of Chemical Substances
CFR	Code of Federal Regulations
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
g/L	grams per litre
g/mL	grams per millilitre
GLP	good laboratory procedure
GRAS	generally recognized as safe

IUPAC	International Union of Pure and Applied Chemistry
kg/m ³	kilogram per cubic metre
KI	Klimisch scoring system
kPa	kilopascal
LC	lethal concentration
mbar	millibar
mg/kg dw	milligrams per kilogram dry weight
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SDES	sodium 2-(2-dodecyloxyethoxy) ethyl sulfate
SGG	Synthetic Greenhouse Gases
USFDA	United States Food and Drug Administration