

**BENZENESULFONIC ACID, DIMETHYL-, SODIUM SALT
[SODIUM XYLENE SULFONATE]**

This dossier on benzenesulfonic acid, dimethyl-, sodium salt (sodium xylene sulfonate) presents the most critical studies pertinent to the risk assessment of sodium xylene sulfonate in its use in drilling muds. It does not represent an exhaustive or critical review of all available data. The majority of information presented in this dossier was obtained from the OECD-SIDS documents on Hydrotropes (which includes sodium xylene sulfonate) (OECD, 2005), and 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 – Sodium xylene sulfonate is classified as a **tier 1** chemical and requires a hazard assessment only.

1 BACKGROUND

Sodium xylene sulfonate is a UVCB substance that is readily biodegradable and does not bioaccumulate. It is expected to have low potential to bind to sediment and soil. Sodium xylene sulfonate is of low toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC): Sodium 3,4-dimethylbenzenesulfonate

CAS RN: 1300-72-7

Molecular formula: C₈H₁₀O₃S.Na

Molecular weight: 208.21 g/mol

Synonyms: Sodium xylene sulfonate; sodium 3,4-dimethylbenzenesulfonate; 3,4-xylenesulfonic acid, sodium salt; sodium dimethylbenzenesulfonate; benzenesulfonic acid, dimethyl; sodium salt

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 Xylene Sulfonate

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	White, crystalline solid	1	ECHA
Melting Point	>300°C @ 101.3 kPa	1	ECHA
Boiling Point	-	-	-
Density	984 kg/m ³ @ 20 °C	1	ECHA
Vapour Pressure	Negligible	2	USEPA, 2017

Property	Value	Klimisch score	Reference
Partition Coefficient (log K_{ow})	-3.12 (measured) @ 20°C	1	ECHA
Water Solubility	664 g/L @ 20°C (pH approximately 11.96)	1	ECHA
Dissociation constant (pKa)	7.1 @ 20°C	1	ECHA

Sodium xylene sulfonate is known as a hydrotrope. Hydrotropes are substances that are amphiphilic, in that they are composed of both a hydrophilic and a hydrophobic functional group. The hydrophobic part of the molecule is a benzene substituted non-polar segment. The hydrophilic polar segment is an anionic sulfonate group that is comparatively a short side chain, accompanied by a counter ion. Hydrotropes are used as coupling agents to solubilise the water-insoluble and often incompatible functional ingredients of household and institutional cleaning products and personal care products. The hydrotropes are not surfactants, but are used to solubilise complex formulas in water (OECD, 2005).

Sodium xylene sulfonate is expected to dissociate completely in aqueous media.

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 xylene sulfonate.

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

Sodium xylene sulfonate is readily biodegradable and it does not bioaccumulate. It is expected to have low potential to bind to sediment and soil.

B. Partitioning

Hydrotropes are not volatile substances and not subject to hydrolysis. Sodium xylene sulfonate is expected to dissociate completely in aqueous media.

C. Biodegradation

Sodium xylene sulfonate is readily biodegradable. In two separate OECD 301B tests, degradation was 74% in 15 days; and 88% and 84% in 28 days. In the second test, the 60% threshold was attained after 6 days (OECD, 2005; 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).

D. Environmental Distribution

No experimental data are available for sodium xylene sulfonate. Using KOCWIN in EPISuite™ (USEPA, 2017), the estimated K_{oc} value of 2,4-dimethylsulfonate and 3,4-dimethylsulfonate from the molecular connectivity index (MCI) and $\log K_{ow}$ are 26.3 and 0.7876 L/kg, respectively. Thus, the potential for adsorption to soil or sediment is low. Based on these values along with the sodium xylene sulfonate's high water solubility, if released to water, it will likely preferentially partition into the water column and not adsorb to suspended solids or sediments.

E. Bioaccumulation

No experimental studies have been conducted on sodium xylene sulfonate. Fish bioconcentration tests (OECD TG 305C) have been conducted on similar substances: sodium xylene sulfonate (CAS No. 827-21-4) and sodium toluene sulfonate (CAS No. 12068-03-0). All measured values were lower than the detection limit of the HPLC analysis. The measured BCF values in *Cyprinus* species were <2.3 (OECD, 2005). Thus the substance does not appreciably bioconcentrate.

6 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

Sodium xylene sulfonate is of low toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 3 lists the results of acute aquatic toxicity studies on sodium xylene sulfonate.

Table 3 Acute Aquatic Toxicity Studies on Sodium Xylene Sulfonate

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Rainbow trout	96-hour LC ₅₀	>408 a.i.*	2	OECD, 2005
Fathead minnow	96-hour LC ₅₀	>400 a.i.	2	OECD, 2005
<i>Daphnia magna</i>	48-hour EC ₅₀	>408 a.i.	2	OECD, 2005

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
<i>Daphnia magna</i>	48-hour EC ₅₀	>400 a.i.	2	OECD, 2005
<i>Selenastrum capricornutum</i>	96-hour EC ₅₀ NOEC	230 31	2	OECD, 2005

*= active ingredient

Chronic Studies

No studies are available.

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).

Sodium xylene sulfonate is readily biodegradable; thus it does not meet the screening criteria for persistence.

The BCF values from two separate fish bioconcentrations on similar substances to sodium xylene sulfonate were <2.3. Thus, sodium xylene sulfonate does not meet the criteria for bioaccumulation.

The NOEC from an algal study on sodium xylene sulfonate is >0.1 mg/L. The acute E(L)C₅₀ values for sodium xylene sulfonate are >1 mg/L for fish, invertebrates and algae. Thus, sodium xylene sulfonate does not meet the screening criteria for toxicity.

The overall conclusion is that sodium xylene sulfonate is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for sodium xylene sulfonate.

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 Xylene Sulfonate	1300-72-7	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:

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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USEPA. (2017). EPISuite™ v. 4.11, United States Environmental Protection Agency, Office of Pollution Prevention and Toxics and Syracuse Research Corporation. Available at: <https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface>.

B. Abbreviations and Acronyms

°C	degrees Celsius
a.i.	active ingredient
AICS	Australian Inventory of Chemical Substances
BCF	bioconcentration factor
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
HPLC	High performance liquid chromatography
IUPAC	International Union of Pure and Applied Chemistry
kg/m ³	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L/kg	litres per kilogram
LC	lethal concentration
MCI	molecular connectivity index
mg/L	milligrams per litre
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
SGG	Synthetic Greenhouse Gases
SIDS	screening information data set
TG	test guideline