Qualitative Tier 2 Assessment

C10-C16 Alkylbenzenesulfonic Acid

In accordance with the Dawson River Release (DRR) Chemical Risk Assessment Framework (CRAF), chemicals assigned a Tier 2 designation require a hazard assessment and qualitative assessment of risk.

Consistent with National Industrial Chemicals Notification and Assessment Scheme (NICNAS), the human health hazards for each chemical are characterised by analysing the toxicokinetics (the absorption, distribution, metabolism and excretion of the chemical in humans or laboratory animals), acute toxicity, irritation and corrosivity, repeat dose toxicity, genotoxicity, carcinogenicity, reproductive toxicity, and other health effects. The environmental hazards for each chemical are characterized by analysing the environmental fate properties (such as mobility, persistence, bioavailability and bioaccumulation), acute toxicity and chronic toxicity. In support of the hazard assessment, a risk assessment dossier is prepared for each of the chemicals included in the assessment.

Potentially complete exposure pathways (in that a source, a migration pathway, a mechanism for exposure, and a potential receptor are present) are qualitatively assessed herein to determine the potential for risk. An incomplete pathway precludes an exposure occurring and an associated potential risk. In this context, site setting and management protocols associated with the action are evaluated. Key controls limiting the potential for exposure include:

- Engineering controls (including fencing and secondary containment);
- Storage (drums, totes and storage tanks) constructed in accordance with Australian standards and managed and monitored in accordance with regulatory requirements;
- Maintenance of access control restrictions during site activities that will preclude access by the public, livestock and large native fauna; and,
- Safe Work Australia and Santos Occupational Safety Guidance used to minimise human health exposure.

This qualitative assessment provides information to be used as a complement to the risk assessment dossier to provide a summary of human and ecological hazards that may occur from exposure to the chemical. Where a potential hazard exists, additional information is provided in the risk assessment dossiers and safety data sheets (SDSs) and are available to emergency responders, health and safety managers, and environmental hazard clean-up teams.

As a result, the assessment for this Tier 2 chemical includes the following components: completing the screening; developing a risk assessment dossier and Predicted No Effect Concentrations (PNECs) for water and soil; and, providing a qualitative discussion of risk. Each of these components is detailed within this memorandum.

Background

Santos has been releasing treated water to the Dawson River since 2015. The Dawson River Release Scheme[1] is located in the southeast region of the Fairview Arcadia Project Area (FAPA) (within the hub compressor station four (HCS4) gathering network). Coal seam water produced in the HCS4 gathering network is collected and is treated at Reverse Osmosis Plant 2 (ROP2) with the treated permeate stored within a permeate pond prior to release to the Dawson River. The outfall location is located within a tributary gully of the Dawson River, which joins the Dawson River midway between "Dawson's Bend" and Yebna Crossing.

The permeate pond is connected to the outfall location by a 5.3-kilometre (km) pipeline constructed across farmland with the released water flowing down a 2.9 km tributary gully before discharging to the Waterbody (nominal capacity 500 megalitre [ML]) and then flowing 1.8 km before joining the Dawson River at its downstream confluence.

ROP 2 at FAPA is a reverse osmosis plant with a specification designed to produce high quality water for the intended release of treated coal seam water to the Dawson River. The process removes the suspended and dissolved solids through a set of six processes to produce high quality treated water. These include coagulation/clarification, oxidation, filtration, softening, reverse osmosis, and finally adjustment of sodium adsorption ratio (SAR).

C10-C16 alkylbenzenesulfonic acid is a component in the KCl/Polymer Stuck Pipe Mud system. The secondary mud system is used to free stuck pipes and, as a secondary mud, will only be used as required. As a result, these secondary muds are considered insignificant relative to the primary muds due to the considerably reduced volume used (<0.1%) as compared to the other muds. The purpose and maximum quantity (i.e., in all muds) for this chemical is summarised in **Table 1**.

Table 1 Drilling Fluid Chemicals

Chemical Name	CAS No.	Use	Quantity[1]
C10-C16 Alkylbenzenesulfonic acid	68584-22-5	Emulsifier	NA

[1] Based on maximum of combined muds assessed
CAS No = Chemical Abstracts Service Number
NA = quantity used varies with severity of loss

The assessment of toxicity of this chemical was used to evaluate human health exposure scenarios and is presented in **Attachment 1**. There are no carcinogenicity studies on C10-C16 alkylbenzenesulfonic acid, and, as a result, only a non-carcinogenic oral reference dose (RfD) was calculated. A detailed discussion of the derivation of the oral RfD and drinking water guideline values is presented in the attachment. **Table 2** provides a summary of the derivation.

[1] Santos obtained an amendment to the Fairview Arcadia Project Area (FAPA) Environmental Authority (EA) (EPPG00928713) on 31st May 2013 to authorise the release of desalinated produced water from the Fairview reverse osmosis plant (ROP) 2 to the Dawson River – the Dawson River Release Scheme (DRRS).

Table 2 Oral Reference Doses and Derived Drinking Water Guidelines

Constituent (CAS No.)	Study	Critical Effect/ Target Organ(s)	NOAEL (mg/kg-day)	Uncertainty Factors	Oral Reference Dose (mg/kg-day)	Drinking Water Guideline (mg/L)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	2-year rat dietary	None	250	100	2.5	9

Refer to **Attachment 1** for information on the key studies selected for oral reference dose and drinking water level development.
CAS = Chemical Abstracts Service
mg/kg-day = milligram per kilogram-day
mg/L = milligram per litre
NOAEL = No observed adverse effect level

For ecological receptors, the assessment utilises the information presented in the dossiers on the relative toxicity of the aquatic and terrestrial flora and fauna to the chemical. This assessment focuses on the aquatic invertebrate and fish species within the surface water resources and the soil flora and fauna associated with releases to the soil.

The determination of toxicological reference values (TRVs) was conducted according to the PNEC guidance in the *Environmental Risk Assessment Guidance Manual for Industrial Chemicals* prepared by the Australian Environmental Agency (AEA, 2009). PNECs for freshwater and sediment were developed to assess aquatic receptors, and PNECs for soil were developed for terrestrial receptors.

Table 3 present the chemical, the endpoint, no observable effects concentration (NOEC) (milligrams per litre [mg/L]), assessment factor, and the aquatic PNEC (mg/L). PNECs for sediment and soil are detailed in **Tables 4** and **5,** respectively. Refer to **Attachment 1** for the development of PNECs, or the rational for PNECs that do not have a calculated PNEC.

Table 3 PNECs Water – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/L)	Assessment Factor	$PNEC_{water}$ (mg/L)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	-	-	-	0.28[a]

[a] $PNEC_{water}$ for C10-C16 alkylbenzenesulfonic acid is the ANZG Water Quality Guideline – Freshwater Trigger Value for Linear Alkylbenzene Sulfonate.
EC_{50} = effects concentration – 50%
mg/L = milligram per litre
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 4 PNECs Sediment – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg wet wt)	Assessment Factor	$PNEC_{sed}$ (mg/kg wet wt)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	[a]	-	-	27

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg wet wt = milligram per kilogram wet weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

Table 5 PNECs Soil – Tier 2 Chemicals

Constituents	Endpoint	EC_{50} or NOEC (mg/kg dry wt)	Assessment Factor	$PNEC_{soil}$ (mg/kg dry wt)
C10-C16 Alkylbenzenesulfonic acid (68584-22-5)	[a]	-	-	24

[a] Calculated using equilibrium partitioning method
EC_{50} = effects concentration – 50%
mg/kg dry wt = milligram per kilogram dry weight
NOEC = no observable effects concentration
PNEC = predicted no effect concentration
Refer to **Attachment 1** for information on the development of PNECs listed above.

A detailed assessment of the risks posed by this Tier 2 chemical is provided in the following sections.

General Overview

C10-C16 alkylbenzenesulfonic acid has an average alkyl chain length of 11.3 to 11.8 (HPVIS). This range includes benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives sulfonic acid (CAS No. 85536-14-7). The molecular structure of C10-C16 alkylbenzenesulfonic acid is presented in **Figure 1**.

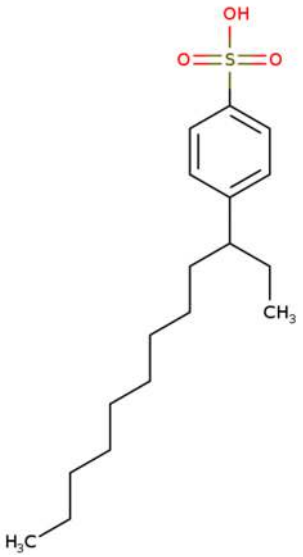

Figure 1 Molecular Structure of C10-C16 Alkylbenzenesulfonic Acid[2]

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. It has a low-to-moderate potential for bioaccumulation based on structurally similar compounds.

The Persistent, Bioaccumulative and Toxic (PBT) assessment for C10-C16 alkylbenzenesulfonic acid is included in the dossier provided in **Attachment 1**. Based on physico-chemical properties and screening data detailed below, the overall conclusion was that C10-C16 alkylbenzenesulfonic acid is not a PBT substance.

Human Health Hazards

C10-C16 alkylbenzenesulfonic acid exhibits moderate acute toxicity by the oral route and low acute toxicity by the dermal route. The following information was derived from products of similar structure or composition. It is highly irritating to the skin and eyes, but not a skin sensitiser. No systemic, reproductive or developmental toxicity was seen. It is not genotoxic.

There are no repeated-dose toxicity studies on C10-C16 alkylbenzenesulfonic acid. However, a reliable two-year dietary study was conducted in rats on C10-C14 Linear Alkylbenzene Sulfonate (CAS No. 69669-44-9). In this study, there were no treatment-related effects with a no observed adverse effect level (NOAEL) of 250 milligrams per kilogram-day (mg/kg-day) (Buehler et al., 1971). This NOAEL was used for determining the oral RfD and the drinking water guideline value (9 mg/L) (see **Table 2**). Description of the oral RFD and calculation of the drinking water guideline value is included in the dossier provided in **Attachment 1**.

C10-C16 alkylbenzenesulfonic acid may be present in treated water (permeate). Managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As the Dawson River meanders through large areas that are uncontrolled, exposures could potentially occur to downstream agricultural workers and residents.

[2] Source https://chem.nlm.nih.gov/chemidplus/rn/68584-22-5

There is low potential for human receptors to be exposed to C10-C16 alkylbenzenesulfonic acid in Dawson River discharge. The combination of mixing/dilution, storage (and associated biodecay) prior to treatment, treatment and retention (and associated biodecay) following treatment are all key components that will reduce the potential risk to potential receptors from discharges to surface water. For example, the concentration of residual chemicals in flowback water would be diluted by at least 90% in the water feed pond due to the aggregation of produced water from other wells within one pond. During water treatment, concentrations would be further reduced by efficiencies of the reverse osmosis system. In addition, C10-C16 alkylbenzenesulfonic acid is readily biodegradable in the environment with a half-life substantially less than 60 days (**Attachment 1**). Estimated concentrations in treated water (refer **Attachment 2**) are less than the derived drinking water guideline value of 9 mg/L.

Finally, there are no public access points to Dawson River within 1.4 km downstream of the most downstream release location, and while there may be some fishing by local landowners in this reach, other forms of secondary recreation are unlikely. Currently, there is no irrigation in the immediate vicinity of the Waterbody, with the closest irrigation being approximately 5km to the west. There is a water supply scheme in the Dawson River that supplies irrigators but this is located 250 km downstream, with a search of the Department of Natural Resources, Mines and Energy (DNRME) now Department of Resources (DoR), database indicating that the nearest licensed surface water take for irrigation is 71 km downstream noting this licence provides authority to extract from an 'Unnamed tributary of the Dawson River', not the Dawson River. The nearest surface water domestic water supply entitlement is 244 km downstream (AECOM, 2019).

Environmental Hazards

In standard aquatic toxicity tests, C10-C16 alkylbenzenesulfonic acid is a moderate toxicity concern to aquatic organisms. Acute toxicity towards fish and aquatic invertebrates is of the same order of magnitude. However, algae (*Scenedesmus subspicatus)* was somewhat less sensitive (ECHA).

C10-C16 alkylbenzenesulfonic acid is biodegradable and does not persist in the environment. The chemical also has a low potential for bioaccumulation.

PNECs for C10-C16 alkylbenzenesulfonic acid are provided in **Tables 3 – 5**. The C10-C16 alkylbenzenesulfonic acid is a Linear Alkylbenzene Sulfonate (LAS). ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 0.28 mg/L for LAS. This value, which was identified as the PNEC for water (see **Table 3**), was derived using data normalised to an alkyl chain length of C11.6 using the statistical distribution method with 95% protection.

There are no toxicity data for sediment-dwelling organisms or soil organisms. Therefore, PNECs for sediment and soil were calculated using the equilibrium partitioning method (see **Tables 4 and 5**). PNEC calculations and assumptions are detailed in the dossier provided in **Attachment 1**.

As described in the previous section (Human Health Hazards), managed release of treated water to the Dawson River would have the potential to affect surface water within the river. As released treated water would become part of the regional surface water resource (i.e., Dawson River water quality and flow), ecological resources (livestock and native flora and fauna) are potential receptors. Specifically, potential receptors include:

- Aquatic ecological receptors within Dawson River downstream of the release point
- Livestock and wildlife that may access Dawson River surface water

Stock access to large portions of the Waterbody is permitted and has been observed. The banks of the Waterbody are severely degraded and lack riparian vegetation due to cattle access/activity. Similarly, cattle access the Dawson River for water at numerous places within and downstream of the receiving environment (frc environmental, 2021).

There is limited extraction of water for general farm supply downstream of the release location to the Dawson River. There is one licensed surface water take for agriculture within the extent of the release location area. Santos is in regular direct communication with the landholder and is not aware of any abstraction being undertaken under this licence to date. In addition, the nearest downstream agricultural area is located approximately 7 km downstream of the release location to the Dawson River.

Biological monitoring has identified the presence of Matters of National Environmental Significance (MNES) receptor white-throated snapping turtle (*Elseya albagula*) in two upstream locations (at site DRR2 on Hutton Creek and at site DRR1 on Dawson River). The presence of MNES receptor Fitzroy River Turtle (*Rheodytes leukops*) has not been identified.

The potential for exposure of sensitive receptors, including MNES, is low. Released treated water mixes with surface water in a manner that is protective of aquatic receptors within the Dawson River (AECOM, 2019). Treated water releases from the permeate ponds are less than 18 megalitre (ML)/day with Santos undertaking periodic releases. Releases are currently dictated by treated effluent production rates. Perennial base flow in the Dawson River downstream of Dawson's Bend at the Dawson River discharge point has been assessed as 21 ML/day. Baseflow in the Dawson River is associated with spring discharges.

Further, quantitative mass balance calculations of C10-C16 alkylbenzenesulfonic acid in treated water demonstrate theoretical concentrations less than PNECs for aquatic receptors (refer **Attachment 2**). The potential exposure point concentrations (EPCs) have been conservatively estimated. As detailed in **Attachment 2**, a quantitative mass balance calculation was undertaken to identify the amount of C10-C16 alkylbenzenesulfonic acid in recovered drilling fluids. Residual fluids that are not recycled are transferred to the WMF. These fluids (10% by volume) were diluted in the Water Management Facility (WMF) water feed pond influent by wells that did not contain detectable concentrations of this constituent. This EPC was then adjusted based on biodegradation rates to calculate the theoretical EPCs for two exposure time periods (0 and 30 days) which represent no storage/no degradation (Day 0) and a bounding estimate which considers degradation during storage at the WMF. Chemicals that are readily biodegradable, such as C10-C16 alkylbenzenesulfonic acid, are not persistent and may only be present in the aquatic compartment for a short period of time. Therefore, consistent with risk assessment guidance (DoEE, 2017), it was assumed that the half-life of this chemical was 15 days.

The concentrations in the water feed pond were then reduced by a factor of 99% to account for efficiencies in the WMF system. Finally, a dilution factor of 50 was assumed to account for dilution into the receiving water body. This factor was based on the approved mixing zone described in the Santos 2013 report *Dawson River Release Scheme – Environmental Authority Amendment Application –Supporting Information*.

References

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Santos, 2013. Dawson River Release Scheme – Environmental Authority Amendment Application – Supporting Information. May 2013.

HPVIS. United States Environmental Protection Agency High Production Volume Information System (HPVIS): https://iaspub.epa.gov/oppthpv/public_search.html_page.

Attachment 1 Risk Assessment Dossier

C10 –C16 ALKYLBENZENESULFONIC ACID

This dossier on C10-C16 alkylbenzenesulfonic acid presents the most critical studies pertinent to the risk assessment of C10-C16 alkylbenzenesulfonic acid in its use incoal seam gas extraction activities . 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 United States Environmental Protection Agency High Production Volume Information System (HPVIS) Chemical Challenge Program. Where possible, study quality was evaluated using the Klimisch scoring system (Klimisch *et al.*, 1997).

Screening Assessment Conclusion – C10-C16 alkylbenzenesulfonic acid was not identified in chemical databases used by NICNAS as an indicator that the chemical is of concern and is not a PBT substance. C10-C16 alkylbenzenesulfonic acid was assessed as a tier 2 chemical for acute toxicity. Therefore, C10-C16 alkylbenzenesulfonic acid is classified overall as a **tier 2** chemical and requires a hazard assessment and qualitative assessment of risk.

1 BACKGROUND

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. It has a low-to-moderate potential for bioaccumulation based on structurally similar compounds. C10-C16 alkylbenzenesulfonic acid exhibits moderate acute toxicity by the oral route and low acute toxicity by the dermal route. The following information was derived from products of similar structure or composition. It is highly irritating to the skin and eyes, but not a skin sensitiser. Repeated oral toxicity studies have shown no target organ effects. It is not genotoxic, and animal dietary studies showed no indication of adverse reproductive or developmental effects. C10-C16 alkylbenzenesulfonic acid is of moderate toxicity concern to aquatic organisms.

2 CHEMICAL NAME AND IDENTIFICATION

Chemical Name (IUPAC):
petroleum, di-C10-16 linear saturated alkaryl derivatised Benzenesulfonic acids
CAS RN: 68584-22-5
Molecular formula: variable
Molecular weight: variable

Synonyms: p-dodecylbenzenesulfonic acid; Benzenesulfonic acid, 4-dodecyl-4-Dodecylbenzene-1-sulfonic acid; 4-Dodecylbenzenesulphonic acid (mixed isomers)

C10-C16 alkylbenzenesulfonic acid (CAS No. 68584-22-5) has an average alkyl chain length of 11.3 to 11.8 (HPVIS). This range includes benzenesulfonic acid, 4-C10-13-sec-alkyl derivs. sulfonic acid (CAS No. 85536-14-7).

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 C10-C16 Alkylbenzenesulfonic Acid

Property	Value	Klimisch score	Reference
Physical state at 20°C and 101.3 kPa	Brown, viscous liquid	-	ECHA
Melting Point	334 °C @ 101.3 kPa	2	ECHA
Boiling Point	1043 °C @ 101.3 kPa	2	ECHA
Density	-	-	-
Vapor Pressure	2.89 x 10^{-8} Pa (estimated) (temperature not provided)	2	HPVIS
Partition Coefficient (log K_{ow})	22 @ 25°C	2	ECHA
Water Solubility	0 g/L @ 25°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 C10-C16 alkylbenzenesulfonic acid.

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

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. It is insoluble in water and has a high potential for adsorption to soil or sediments. It has a low-to-moderate potential for bioaccumulation based on structurally similar compounds.

B. Partitioning

Based on its vapour pressure, volatilisation is not expected to be an important fate and transport pathway.

C. Biodegradation

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable. In an OECD DOC Die-away test, benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) was degraded 94% after 28 days (HPVIS) [Kl. score = 1]. In a modified coupled units test, benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) was degraded 92% after 37 days (HPVIS) [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 studies are available for C10-C16 alkylbenzenesulfonic acid. Using KOCWIN in EPISUITE™ (USEPA, 2017), the estimated K_{oc} values for various surrogates of C10-C16 alkylbenzenesulfonic acids are presented in Table 3 which indicate that these compounds are expected to have the potential for low to slight mobility or even immobility (Koc >5,000) in soil. I If released to water, based on these K_{oc} values and the substance's insolubility, it would likely also adsorb to suspended solids or sediment.

Table 3 K_{oc} Values for Surrogates of C10-C16 Alkylbenzenesulfonic Acid

Substance	K_{oc} (MCI estimate)	K_{oc} (log K_{ow} estimate)
4-(1-ethyloctyl)-benzenesulfonic acid	3,505 L/kg	973.4 L/kg
4-(1-ethylnonyl)-benzenesulfonic acid [CAS No. 18777-52-1]	6,388 L/kg	1,817 L/kg
4-(1-ethyltetradecyl)-benzenesulfonic acid	128,400 L/kg	41,690 L/kg

E. Bioaccumulation

No experimental studies are available for C10-C16 alkylbenzenesulfonic acid. Bioconcentration of C10-C16 alkylbenzenesulfonic acid in aquatic organisms is not expected to occur based on a measured log K_{ow} of 2.0 (HPVIS).

A bioconcentration fish (OECD 305 E) study was conducted on C10-C13 Linear Alkylbenzene Sulfonate (LAS). The BCF values ranged between 2 and 1,000 L/kg, with BCFs increasing with increasing alkyl chain length. To address differences in composition of mixtures, bioconcentration potential was evaluated for a mixture typical of LAS in European detergent formulations (C10 12%, C11 29%, C12 34%, C13 24%); average alkyl chain length – C11.6 and a mixture typical of LAS in filtered Mississippi river water (C10 45%, C11 23%, C12 23%, C13 2%; average chain length = C10.8). The respective BCFs were 87 and 22 L/kg at concentrations of 2.7 and 4.1 µM (HPVIS). [Kl. score = 2]

A BCF of 130 was reported for *Leuciscus idus melanotus* in a 3-day test conducted on dodecylbenzenesulfate, sodium salt (HPVIS). [Kl. score = 1]

6 HUMAN HEALTH HAZARD ASSESSMENT

A. Summary

C10-C16 alkylbenzenesulfonic acid exhibits moderate acute toxicity by the oral route and low acute toxicity by the dermal route. The following information was derived from products of similar structure or composition. It is highly irritating to the skin and eyes, but not a skin sensitiser. Repeated oral toxicity studies have shown no target organ effects. It is not genotoxic, and animal dietary studies showed no indication of adverse reproductive or developmental effects.

B. Acute Toxicity

The oral LD_{50} in rats for the C10-C16 alkylbenzenesulfonic acid is 775 mg/kg (HPVIS) [Kl. score = 1]. The oral LD_{50} in rats for the benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) is 1,470 mg/kg (HPVIS). [Kl. score = 1]

The dermal LD_{50} in rabbits for C10-C16 alkylbenzenesulfonic acid is 2,000 mg/kg (HPVIS). [Kl. score = 1]

C. Irritation

No studies are available on C10-C16 alkylbenzenesulfonic acid.

Application of 0.5 mL benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) to the skin of rabbits for four hours was highly irritating. The irritation index was 5.25 (HPVIS). [Kl. score = 1]

Instillation of 0.1 ml benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7) into the eyes of rabbits was moderately irritating. The primary irritation index was 46.9 (HPVIS). [Kl. score = 1]

D. Sensitisation

No studies are available on C10-C16 alkylbenzenesulfonic acid.

A C10-C13 benzenesulfonic acid was not considered a skin sensitiser in a guinea pig maximisation test (HPVIS). [Kl. score = 1]

E. Repeated Dose Toxicity

No studies are available for C10-C16 alkylbenzenesulfonic acid.

Oral

Male and female Wistar rats were given feed containing 0, 0.07, 0.2, 0.6 or 1.8% C10-C14 alkylbenzenesulfonic acid for six months. The 1.8% group had diarrhea, markedly depressed growth, increased cecal weight and marked degeneration of the renal tubules. The 0.6% group had slightly depressed growth, increased cecal weight, increased serum alkaline phosphatase activity, decreased serum protein and degeneration of the renal tubules. The 0.2% group had increased cecal weight and slight degeneration of the renal tubules. The 0.07% group showed no treatment-related effects. The NOAEL was reported to be 0.07%, which was estimated to be 40 mg/kg-day (Yoneyama *et al.*, 1972; IPCS 1996). [Kl. score = 4]

Male and female Wistar rats were given feed containing 0, 0.04, 0.16 or 0.6% C10-C14 alkylbenzenesulfonic acid for up to 24 months. The 0.6% group had slightly increased live and cecal weights, and increased activity of serum glutamate-pyruvate transaminase and alkaline phosphatase. There were no treatment-related effects on food consumption, body weight gain, clinical signs, mortality or mean survival. The NOAEL was considered to be 0.6%, which was estimated to be 300 mg/kg-day (Yoneyama et al., 1977; IPCS, 1996). [Kl. score = 4]

Male and female CR rats were given feed containing 0, 0.02, 0.1 or 0.5% C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9) for two years. The mean daily intakes were estimated to be 0, 10, 50 and 250 mg/kg-day. Body weight gain and feed consumption were similar across all groups. There were no treatment-related effects on hematology parameters in the gross pathology or histopathology examination. The NOAEL is 250 mg/kg-day (Buehler et al., 1971; HPVIS). [Kl score = 2]

Inhalation

No studies are available.

Dermal

No studies are available.

F. Genotoxicity

In Vitro Studies

C10-C16 alkylbenzenesulfonic acid was not mutagenic to *S. typhimurium* strains TA98 and TA100 in the absence or presence of metabolic activation (HPVIS). [Kl. score = 1]

In Vivo Studies

Male and female NMRI mice were dosed by oral gavage with a single dose of 0 or 1,122 mg/kg benzenesulfonic acid, C10-C13 alkyl derivatives (CAS No. 85536-14-7). There were no significant increases in the number of micronucleated polychromatic erythrocytes in bone marrow cells (HPVIS). [Kl. score = 1]

Male and female ICR: JCL mice were dosed by oral gavage with 0, 200, 400 or 800 mg/kg C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9) either as a single dose or given a single daily dose for 5 consecutive days. There were no significant increases in the number of chromosomal aberrations in bone marrow cells (HPVIS). [Kl. score = 1]

G. Carcinogenicity

Oral Studies

No studies are available on C10-C16 alkylbenzenesulfonic acid.

Male and female CR rats were given feed containing 0, 0.02, 0.1 or 0.5% C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9) for two years. The mean daily intakes were estimated to be 0, 10, 50 and 250 mg/kg-day. Body weight gain and feed consumption were similar across all groups. The incidence of tumours in the treated animals were similar to the controls (Buehler et al., 1971; HPVIS). [Kl score = 2]

H. Reproductive Toxicity

No studies are available on C10-C16 alkylbenzenesulfonic acid.

A reproductive toxicity study was conducted on C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9). The dietary doses were 0, 0,02, 0.1 or 0.5%, which were estimated to be 0, 14, 70 and 350 mg/kg-day, respectively. The P0 generation were fed for 84 days; when 107-112 days old, females from each dose group were mated with males from the same group and maintained together for 17 days. The first litters of each generation (F1a- and F2a-generation) were sacrificed at 21 days of age. Ten days after the final litter was sacrificed, all females were re-mated with different males from the same group to obtain the F1b generation. From the F1b generation, males and females of each group were selected at weaning to continue their respective diets and to be used for further reproduction studies. Reproduction studies on the F1b and F2b generations were started when the rats were 80-85 days old, and were continued until the F3b generation was weaned. There were no treatment-related effects on fertility, gestation, parturition, neonatal viability, lactation, and post-weaning growth. The NOAEL for reproductive toxicity is 350 mg/kg-day, the highest dose tested (Buehler et al., 1971; HPVIS). [Kl. score = 2]

I. Developmental Toxicity

No studies are available on C10-C16 alkylbenzenesulfonic acid.

Pregnant female SD-JCL rats were given in their feed 0, 0.1 or 1.0% Linear Alkylbenzene Sulfonate (average alkyl chain length = C11.7 to C12.3) on GD 0 to 20. Body weight gain in the dams were similar between treated and control groups, and there was no treatment-related effects on the occurrence and maintenance of pregnancy. The litter parameter values were similar across all groups and there was no evidence of teratogenicity. In the 1% group, the numbers of offspring were low and the weaning rate was 78.3% compared to the rate in the controls (100%). There were no adverse effects in the offspring body weight gain, organ weights or function. The NOAEL for

maternal and developmental toxicity is considered to be 1% in the diet (calculated to be 780 mg/kg-day) (Tiba et al., 1976; HPVIS). [Kl. score = 4]

J. Derivation of Toxicological Reference and Drinking Water Guidance Values

The toxicological reference values developed for C10-C16 alkylbenzenesulfonic acid follow the methodology discussed in enHealth (2012). The approach used to develop drinking water guidance values is described in the Australian Drinking Water Guidelines (ADWG, 2011).

Non-Cancer

Oral

There are no repeated-dose toxicity studies on C10-C16 alkylbenzenesulfonic acid (CAS No. 68584-22-5). However, a reliable (Kl. score = 2) two-year dietary study was conducted in rats on C10-C14 Linear Alkylbenzene Sulfonate (CAS No. 69669-44-9). In this study, there were no treatment-related effects with a NOAEL of 250 mg/kg-day (Buehler et al., 1971 as cited in OECD 2005). This study is supported by another two-year rat dietary study conducted on C10-C14 alkylbenzenesulfonic acid, which was published in a Japanese journal and was summarised in IPCS (1996); the NOAEL from this study was considered to be 300 mg/kg-day.

The NOAEL of 250 mg/kg-day from Buehler *et al.*, (1971) (as cited in OECD 2005) will be used for determining the oral Reference Dose (RfD) and the drinking water guidance value.

Oral Reference Dose (oral RfD)

Oral RfD = NOAEL / (UF_A x UF_H x UF_L x UF_{Sub} x UF_D)

Where:
UF_A (interspecies variability) = 10
UF_H (intraspecies variability) = 10
UF_L (LOAEL to NOAEL) = 1
UF_{Sub} (subchronic to chronic) = 1
UF_D (database uncertainty) = 1

Oral RfD = 250/(10 x 10 x 1 x 1 x 1) = 250/100 = 2.5 mg/kg-day

Drinking water guidance value

Drinking water guidance value = (animal dose) x (human weight) x (proportion of intake from water) / (volume of water consumed) x (safety factor)

Using the oral RfD,

Drinking water guidance value = (oral RfD) x (human weight) x (proportion of water consumed) / (volume of water consumed)

Where:
Human weight = 70 kg (ADWG, 2011)
Proportion of water consumed = 10% (ADWG, 2011)
Volume of water consumed = 2L (ADWG, 2011)

Drinking water guidance value = (2.5 x 70 x 0.1)/2 = 9 mg/L

Cancer

No carcinogenicity studies are available on C10-C16 alkylbenzenesulfonic acid. However, a chronic dietary study was conducted in rats on C10-C14 linear alkylsulfonate, sodium salt (CAS No. 69669-44-9), which has a similar composition to C10-C16 alkylbenzenesulfonic acid. There were no carcinogenic effects in this dietary study. Therefore, a cancer reference value was not derived.

K. Human Health Hazard Assessment of Physico-Chemical Properties

C10-C16 alkylbenzenesulfonic acid does not exhibit the following physico-chemical properties:

- Explosivity
- Flammability
- Oxidising potential

7 ENVIRONMENTAL EFFECTS SUMMARY

A. Summary

C10-C16 alkylbenzenesulfonic acid is of moderate toxicity concern to aquatic organisms.

B. Aquatic Toxicity

Acute Studies

Table 4 lists the results of acute aquatic toxicity studies conducted on C10-C16 alkylbenzenesulfonic acid.

Table 4 Acute Aquatic Toxicity Studies on C10-C16 Alkylbenzenesulfonic Acid

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Cyprinus carpio	96-hour LC_{50}	5.6*	1	HPVIS
Daphnia magna	48-hour EC_{50}	5.2*	1	HPVIS
Daphnia magna	48-hour EC_{50}	9.3 – 11.6**	1	HPVIS
Daphnia magna	48-hour EC_{50}	2.9	1	HPVIS

Test Species	Endpoint	Results (mg/L)	Klimisch score	Reference
Scenedesmus subspicatus	72-hour EC_{50}	36* (growth rate)	1	HPVIS
Scenedesmus subspicatus	EC_{50}	170***	1	HPVIS

*Benzenesulfonic acid, C10-C13-alkyl derivatives

**Three Linear Sulfonic Acids (LAB) of varying chain lengths were neutralised with caustic soda to obtain the sodium salt derivative. Acid A had 48.4% of its weight in the C11 range and the majority of its chain length ranged from C10-C13. Acid B had a 49.4% of its weight in the C11 range and 31.7% of its weight in the C12 range. The majority of its chain length ranged from C10 to C12. Acid C had the majority of its chain length in the C10 to C13 range, almost evenly distributed between C11 and C12. The LC_{50} values were 11.6, 10.8 and 9.3 for Acids A, B and C, respectively.

***C10-C13 linear alkyl benzenesulfonic acid

Chronic Studies

The 28-day chronic toxicity of a commercial C10-C13 Linear Alkylbenzene Sulfonate (average carbon lengths of C11.6 and C11.8) was tested in several species of fish. The NOEC values were normalised using QSARs to the average structure of C11.6 Linear Alkylbenzene Sulfonate. The geometric mean NOECs (and the number of studies) for the various fish species are as follows: 2.3 mg/L for *Brachydanio rerio* (n=1); 0.87 mg/L for *Pimephales promelas* (n=14); 0.34 mg/L for *Oncorhynchus mykiss* (n=7); and 0.25 mg/L for *Tilapia mossambica* (n=1) (HPVIS). [Kl. score = 4].In a chronic *Daphnia* study, the NOEC of the geometric mean of 12 records compiled from the literature review and the LAS normalised to C11.6 was 1.4 mg/L (HPVIS). [Kl. score = 4]. The low Klimisch ratings for these studies make them unsuitable for risk categorization.

C. Terrestrial Toxicity

No adequate information is available.

D. Calculation of PNEC

The PNEC calculations for C10-C16 alkylbenzenesulfonate follow the methodology discussed in DEWHA (2009).

PNEC water

The C10-C16 alkylbenzenesulfonate is a Linear Alkylbenzene Sulfonate (LAS).

ANZG has established a water quality guideline (ANZG, 2018) with a freshwater trigger value of 280 µg/L for LAS. This value was derived using data normalised to an alkyl chain length of C11.6 using the statistical distribution method with 95% protection.

The data set that was used included the following:

Freshwater fish: 5 species, 250 to 3,200 µg/L.

Freshwater crustaceans: 2 species, 1,400−3,200 µg/L.

Freshwater insects: 2 species, 2,800−3,400 µg/L.

Freshwater mesocosms: NOEC of 300 µg/L by Guhl and Gode (1989), an OECD guideline study.

Freshwater algae: 6 species, 80−15, 000 µg/L

PNEC sediment

There are no toxicity data for sediment-dwelling organisms. Therefore, the $PNEC_{sed}$ was calculated using the equilibrium partitioning method. The $PNEC_{sed}$ is 27 mg/kg sediment wet weight.

The calculations are as follows:

$PNEC_{sed} = (K_{sed\text{-}water}/BD_{sed}) \times 1000 \times PNEC_{water}$
$= (123.4/1280) \times 1000 \times 0.28$
$= 27$ mg/kg

Where:
$K_{sed\text{-}water}$ = suspended matter-water partition coefficient (m^3/m^3)
BD_{sed} = bulk density of sediment (kg/m^3) = 1,280 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$K_{sed\text{-}water} = 0.8 + [0.2 \times Kp_{sed}/1000 \times BD_{solid}]$
$= 0.8 + [0.2 \times 255.5/1000 \times 2400]$
$= 123.4\ m^3/m^3$

Where:
Kp_{sed} = solid-water partition coefficient (L/kg)
BD_{solid} = bulk density of the solid phase (kg/m^3) = 2,400 [default]

$Kp_{sed} = K_{oc} \times f_{oc}$
$= 6,388 \times 0.04$
$= 255.5$ L/kg

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for C10-C16 alkylbenzenesulfonate calculated from EPISUITE™ using MCI and the surrogate 4-(1-ethylnonyl)-benzenesulfonic acid is 6,388 L/kg. As discussed in Section 5, the K_{oc} value for this substance ranges from 3,505 L/kg to 128,404 L/kg. The PNEC value is directly related to this value. Thus, a lower K_{oc} would result in a lower PNEC and vice versa.
f_{oc} = fraction of organic carbon in sediment = 0.04 [default].

PNEC soil

There are no toxicity data for terrestrial or soil organisms. Therefore, the $PNEC_{soil}$ was calculated using the equilibrium partitioning method. The $PNEC_{soil}$ is 24 mg/kg soil dry weight.

The calculations are as follows:

$PNEC_{soil} = (Kp_{soil}/BD_{soil}) \times 1000 \times PNEC_{water}$
$= (127.8/1500) \times 1000 \times 0.28$
$= 24$ mg/kg

Where:
Kp_{soil} = soil-water partition coefficient (m^3/m^3)
BD_{soil} = bulk density of soil (kg/m^3) = 1,500 [default]
$PNEC_{water}$ = predicted no effect concentration in water

$Kp_{soil} = K_{oc} \times f_{oc}$
$= 6{,}388 \times 0.02$
$= 127.8\ m^3/m^3$

Where:
K_{oc} = organic carbon normalised distribution coefficient (L/kg). The K_{oc} for C10-C16 alkylbenzenesulfonate calculated from EPISUITE™ using MCI and the surrogate 4-(1-ethylnonyl)-benzenesulfonic acid is 6,388 L/kg. As noted, above the K_{oc} value for this substance is variable.
f_{oc} = fraction of organic carbon in soil = 0.02 [default].

8 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 (IChEMS, 2022; ECHA, 2017).

C10-C16 alkylbenzenesulfonic acid is expected to be readily biodegradable; thus it does not meet the screening criteria for persistence.

The experimental BCFs for several linear alkylbenzene sulfonates that are structurally related to C10-C16 alkylbenzenesulfonate range from 22 to 130; thus, C10-C16 alkylbenzenesulfonic acid does not meet the screening criteria for bioaccumulation.

The chronic toxicity data on C10-C16 alkylbenzenesulfonic acid show NOECs of >0.1 mg/L. Thus, C10-C16 alkylbenzenesulfonate does not meet the screening criteria for toxicity.

The overall conclusion is that C10-C16 alkylbenzenesulfonic acid is not a PBT substance.

B. Other Characteristics of Concern

No other characteristics of concern were identified for C10-C16 alkylbenzenesulfonic acid.

9 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]	
C10-C16 alkylbenzenesulfonic acid	68584-22-5	Not a PBT	No	No	No	No	No	No	2	Insufficient data quality for categorisation	2

Footnotes:

1 - PBT Assessment based on PBT Framework.

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

3 - Tier 2 - Hazard Assessment and Qualitative Assessment Only. Develop toxicological profile and PNECs for water and soil and provide qualitative discussion of risk.

Notes:

NA = not applicable

PBT = Persistent, Bioaccumulative and Toxic

B = bioaccumulative

P = persistent

T = toxic

10 REFERENCES, ABBREVIATIONS AND ACRONYMS

A. References

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B. Abbreviations and Acronyms

°C	degrees Celsius
ADWG	Australian Drinking Water Guidelines
AICS	Australian Inventory of Chemical Substances
ANZG	Australian and New Zealand Guidelines
BCF	bioconcentration factor
COC	constituent of concern
DEWHA	Department of the Environment, Water, Heritage and the Arts

DOC	dissolved organic carbon
EC	effective concentration
ECHA	European Chemicals Agency
EU	European Union
GD	Gestational day
HHRA	enHealth Human Risk Assessment
HPV	High Production Volume
HPVIS	High Production Volume Information System
IChEMS	Industrial Chemicals Environmental Management Standard
IUPAC	International Union of Pure and Applied Chemistry
kg	kilogram
kg/m^3	kilograms per cubic metre
KI	Klimisch scoring system
KOCWIN™	USEPA organic carbon partition coefficient estimation model
kPa	kilopascal
L	litre
L/kg	litres per kilogram
LAS	Linear Alkyl Sulfonate
LC	lethal concentration
LD	lethal dose
LOAEL	lowest observed adverse effect level
m^3	cubic metre
MCI	molecular connectivity index
mg/kg	milligrams per kilogram
mg/L	milligrams per litre
mL	millilitre
NICNAS	The National Industrial Chemicals Notification and Assessment Scheme
NOAEL	no observed adverse effect level
NOEC	no observed effective concentration
OECD	Organisation for Economic Co-operation and Development
Pa	pascal
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No Effect Concentration
ppm	parts per million

QSAR	quantitative structure activity relationship
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RfD	Reference Dose
SGG	Synthetic Greenhouse Gases
USEPA	United States Environmental Protection Agency
UVCB	Unknown or Variable Composition, Complex Reaction Products and Biological Materials
µg/L	micrograms per litre
µM	micromolar

Attachment 2 Mass Balance Calculations

Attachment 2
Comparison of Theoretical Concentrations of COPCs to PNECs (Water)

Chemical	CAS No.	Estimated Initial Vendor Chemical Concentration In Drilling Fluids (mg/L)	Half-Life (days)	Estimated Concentration in Combined Balance Water Feed Pond to WMF		Estimated Concentration in Permeate after 99% treatment efficiency by RO plant		Estimated Concentration in Dawson River (Treated Water Release)		PNEC aquatic (mg/L)
				Temporal Scenario (days)		Temporal Scenario (days)		Temporal Scenario (days)		
				0	30	0	30	0	30	
C10-C16 Alkylbenzenesulfonic acid	68584-22-5	1.00E+00	1.50E+01	1.00E-01	2.50E-02	1.00E-03	2.50E-04	2.00E-05	5.00E-06	2.80E-01

Notes:
mg/L = milligrams per liter
CAS = Chemical Abstracts Service
NA = not applicable
PNEC = predicted no effects concentration
RO = reverse osmosis
WMF = Water Management Facility