Australian Government
Department of Health and Aged Care
Australian Industrial Chemicals Introduction Scheme

Long chain (C≥10) alkyl benzene sulfonates

Evaluation statement

22 December 2022

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AICIS evaluation statement

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Long chain (C≥10) alkyl benzene sulfonates

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Reason for the evaluation

Evaluation Selection Analysis indicated a potential human health risk.

Parameters of evaluation

These chemicals are a group of structurally similar long chain (C≥10) alkylbenzenesulfonates (ABS) and alkylbenzenesulfonic acids (ABSA) that are listed on the Australian Inventory of Industrial Chemicals (the Inventory). The chemicals include both linear alkylbenzenesulfonates/sulfonic acids (LAS/LASA) and branched alkylbenzenesulfonates/sulfonic acids (BAS/BASA). This evaluation is a human health risk assessment for all identified industrial uses of these chemicals. These chemicals are expected to have similar critical health effects primarily driven by the alkylbenzene sulfonate anion.

Chemicals, ABSA and ABS previously assessed under the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) are not covered by this evaluation. However, data from these chemicals has been used as part of a read across approach.

Summary of evaluation

Summary of introduction, use and end use

There is currently no specific information about the introduction, use and end use of this group of chemicals in Australia.

Alkylbenzene sulfonates (ABS) are anionic surfactants used in a range of consumer and industrial applications worldwide, predominantly in cleaning products, with global use volumes in the millions of tonnes per year. ABSA are reported to be primarily an intermediate in the production of ABS although use in cosmetic, domestic, and commercial applications have been reported.

Seven chemicals in this group have uses in cosmetic and personal care products. The reported use concentrations are up to 5% which is consistent with the reported concentrations for structurally similar LAS. These chemicals have reported uses up to a concentration of 10% in domestic products. Structurally similar LAS are reported to be present in laundry detergents and cleaners at concentrations up to 25%.

Some chemicals in this group have reported commercial uses in coatings and paints, fillers, plasters, textile and leather finishing products, and in biocidal products.

Human health

Summary of health hazards

The critical health effects for risk characterisation include:

- local effects (skin and eye irritation, and corrosivity).

Chemicals in this group are expected to cause serious eye damage. In several guideline studies in rabbits, structurally similar LAS were not irritating to the eye at concentrations up to 1%, moderately irritating at 5% and severely irritating at 47–50%.

Based on the available data for benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) and structurally similar LASA, ABSA in this group (CAS Nos. 85536-14-7; 11067-81-5; 68411-32-5) are expected to be corrosive to skin. Based on the weight of evidence of available data for these chemicals and structurally similar chemicals, ABS in this group are considered to be skin irritants. The available data on structurally similar LAS suggest that these chemicals are readily absorbed via the oral route. Based on the available data, these chemicals have moderate acute toxicity via the oral route.

Based on the weight of evidence, limited available data, read across data for structurally similar LAS and LASA and in silico data, these chemicals are not expected to be skin sensitisers.

Based on available data and read across data, chemicals in this group are not expected to be genotoxic. There are no carcinogenicity and reproductive/developmental toxicity data for these chemicals.

The cation components, sodium, alkylamines and alkanolamines, as well as morpholine, in its' salt form, are not expected to contribute significantly to the toxicity of these chemicals.

Hazard classifications relevant to worker health and safety

These chemicals satisfy the criteria for classification according to the Globally Harmonized System of Classification and Labelling of Chemicals (GHS) (UNECE 2017) for hazard classes relevant for work health and safety as follows. This evaluation does not consider classification of physical hazards and environmental hazards.

The classification for acute toxicity and serious eye damage applies to all chemicals in this group. The classification for corrosion only applies to ABSA in this groups (CAS Nos. 85536-14-7; 11067-81-5; 68411-32-5). The classification for skin irritation applies to all the other chemicals in the group.

Health hazards	Hazard category	Hazard statement
Acute toxicity	Acute Tox. 4	H302: Harmful if swallowed
Corrosion/skin irritation	Skin Corr. 1	H314: Causes severe skin burns and eye damage
Corrosion/skin irritation	Skin Irrit. 2	H315: Causes skin irritation
Serious damage to eyes/eye irritation	Eye Damage 1	H318: Causes serious eye damage

Summary of health risk

Public

Based on the available use information, the public may be exposed to these chemicals:

- by direct application of these chemicals to the skin and hair
- by incidental skin and eye contact with these chemicals during use of domestic products
- accidental exposure of children to these chemicals, by ingestion from liquid laundry detergent capsules.

The critical health effect of chemicals in this group is skin and eye irritation. Based on use information for related LAS, these chemicals are expected to present in cosmetics at low concentrations (up to 5%) and at high concentrations (up to 25%) in domestic cleaning products and up to 60% in laundry products.

The hazard profile and risks are similar to a large number of surfactants that are extensively used in products, with severity dependent on concentration and pH. The risks are minimised when products are formulated to be non-irritating. Additionally, chemicals in this group are frequently formulated with related chemicals with similar toxicity including alcohol ethoxylates, laureth sulfates and lauryl sulfates. Therefore, the risk may be impacted by the cumulative levels of surfactants. Any controls for these chemicals should be considered as part of a broader review of the management of surfactants in the *Poisons Standard* SUSMP (TGA 2022).

Accidental exposure of children to these chemicals by ingestion and eye and skin contact, has occurred from liquid laundry detergent capsules, leading to adverse effects. In 2013, an Australian Industry Guideline for Labelling & Packaging of Liquid Laundry Capsules was published by industry. In 2015, the Australian Competition & Consumer Commission (ACCC) participated in a joint international campaign on liquid laundry detergent capsule risks. The focus was to raise awareness of laundry pod safety, including developing a consistent set of safety information for parents and carers worldwide. The ACCC records from 2019 indicate that there has not been any reported complaints or incidents of laundry capsule ingestions.

Workers

During product formulation and packaging, dermal, ocular and inhalation exposure might occur, particularly where manual or open processes are used. These could include transfer and blending activities, quality control analysis, and cleaning and maintaining equipment. Worker exposure to these chemicals at lower concentrations could also occur while using formulated products containing these chemicals. The level and route of exposure will vary

depending on the method of application and work practices employed. Good hygiene practices to minimise incidental oral exposure are expected to be in place.

Given the local health effects, these chemicals could pose a risk to workers. Control measures to minimise dermal, ocular and inhalation exposure are needed to manage the risk to workers (see **Proposed means for managing risks** section).

Proposed means for managing risk

Public Health

No specific regulatory controls are recommended for chemicals in this group as part of this evaluation. Any controls for these chemicals should be considered as part of a broader review of the management of surfactants in the *Poisons Standard* (SUSMP) (TGA 2022).

Workers

Recommendation to Safe Work Australia

It is recommended that Safe Work Australia (SWA) update the Hazardous Chemical Information System (HCIS) to include classifications relevant to work health and safety.

Information relating to safe introduction and use

The information in this statement including recommended hazard classifications, should be used by a person conducting a business or undertaking at a workplace (such as an employer) to determine the appropriate controls under the relevant jurisdiction Work Health and Safety laws.

Control measures that could be implemented to manage the risk arising from ocular, dermal and inhalation exposure to these chemicals include, but are not limited to:

- using closed systems or isolating operations
- minimising manual processes and work tasks through automating processes
- adopting work procedures that minimise splashes and spills
- cleaning equipment and work areas regularly
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with these chemicals.

Measures required to eliminate or manage risk arising from storing, handling and using these hazardous chemicals depend on the physical form and how these chemicals are used.

Personal protective equipment should not solely be relied upon to control risk and should only be used when all other reasonably practicable control measures do not eliminate or sufficiently minimise risk.

Model codes of practice, available from the SWA website, provide information on how to manage the risks of hazardous chemicals in the workplace, prepare an SDS and label containers of hazardous chemicals. Your Work Health and Safety regulator should be contacted for information on Work Health and Safety laws and relevant Codes of Practice in your jurisdiction.

Conclusions

The conclusions of this evaluation are based on the information described in this statement.

Considering the proposed means of managing risks, the Executive Director is satisfied that the identified human health risks can be managed within existing risk management frameworks. This is provided that all requirements are met under environmental, workplace health and safety and poisons legislation as adopted by the relevant state or territory and the proposed means of managing the risks identified during this evaluation are implemented.

Note: Obligations to report additional information about hazards under *Section 100* of the *Industrial Chemicals Act 2019* apply.

Supporting information

Grouping rationale

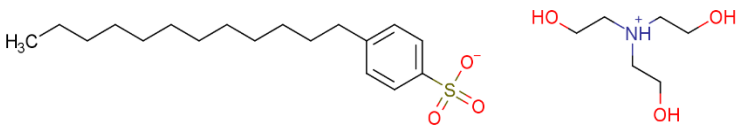
Chemicals in this group are structurally related long chain (C10–60) ABS and ABSA that have surfactant properties. These chemicals include both linear alkyl benzene sulfonates/sulfonic acids (LAS/LASA) and branched alkyl benzene sulfonates/sulfonic acids (BAS/BASA). These chemicals consist of a benzene ring with a sulfonic acid substituent group and an alkyl chain with various chain lengths and distributions. Commercial ABS are UVCBs (unknown or variable composition, complex reaction products or of biological origin) are present as a mixture of homologues and phenyl positional isomers, each containing a sulfonated aromatic ring and an alkyl chain attached at any position except for the sulfonated carbon. There is a higher preponderance at 4- substitutions on the benzene ring over 2-. They are expected to have similar physico-chemical properties, including low water solubility, low vapour pressure, high viscosity, density and melting points. Chemicals in this group have similar end uses, typically as surfactants in domestic and commercial cleaning products.

These chemicals are expected to exist almost entirely as the alkylbenzenesulfonate anion at the pH of biological solutions and therefore are expected to have similar systemic toxicity. The cation components are not expected to contribute significantly to the toxicity of these chemicals. Based on the available data, morpholine and the other amines in their salt forms are not expected to contribute significantly to the toxicity of these chemicals.

These chemicals are surfactants and; therefore, are expected to have similar toxicity on a physico-chemical basis (skin and eye irritation).

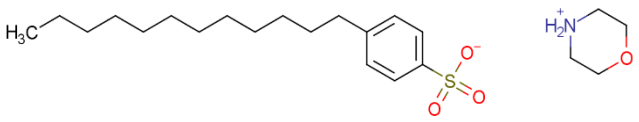
Toxicology information for chemicals in this group is limited. The available data for LAS and LASA with different carbon chain lengths (C10–16) (HERA 2013; NICNAS 2014a; NICNAS 2014b; OECD 2005; US EPA 2014) are used as read across for local and systemic effects. The assessment reports for linear alkylbenzenesulfonates (C10–C16) (NICNAS 2014a) and linear alkylbenzenesulfonic acids (C10–C16) (NICNAS 2014b) should be read in conjunction with this evaluation.

Chemical identity

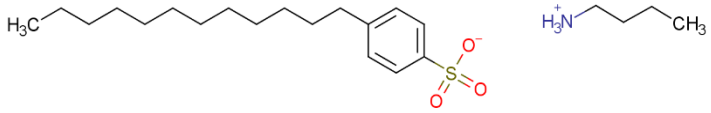
Chemical name	Benzenesulfonic acid, 4-dodecyl-, compound with 2,2',2''-nitrilotris[ethanol] (1:1)
CAS No.	3088-30-0
Synonyms	-
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_6H_{15}NO_3$
Molecular weight (g/mol)	475.7

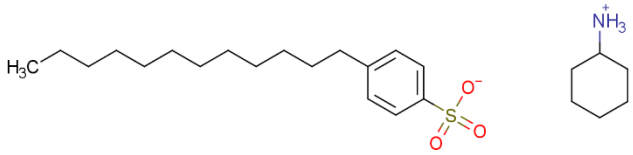
SMILES	OCC[NH+](CCO)CCO.CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

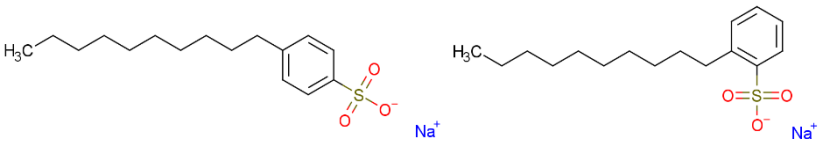
Chemical name	Benzenesulfonic acid, tetrapropylene-
CAS No.	11067-81-5
Synonyms	tetrapropylenebenzenesulfonate
Structural formula	structure not available
Molecular formula	$C_{18}H_{22}O_3S$
Molecular weight (g/mol)	318.4
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, dodecyl-, compound with morpholine (1:1)
CAS No.	12068-08-5
Synonyms	dodecylbenzenesulfonic acid, morpholine salt morpholine, dodecylbenzenesulfonate
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_4H_9NO$
Molecular weight (g/mol)	413.6
SMILES	C1COCC[NH2+]1.CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

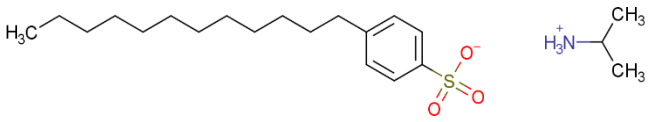
Chemical name	Benzenesulfonic acid, 4-dodecyl-, compound with 1-butanamine (1:1)
CAS No.	14356-36-6
Synonyms	butylamine 4-dodecylbenzenesulfonate (1:1)

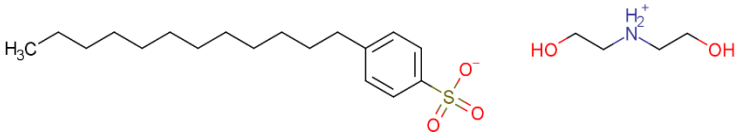
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_4H_{11}N$
Molecular weight (g/mol)	399.6
SMILES	CCCC[NH3+].CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, p-dodecyl-, compound with cyclohexylamine (1:1)
CAS No.	14356-38-8
Synonyms	p-dodecylbenzenesulfonic acid, cyclohexylamine salt
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_6H_{13}N$
Molecular weight (g/mol)	425.7
SMILES	[NH3+]C1CCCCC1.CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

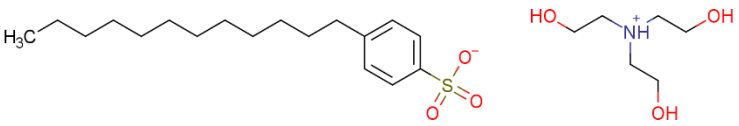
Chemical name	Benzenesulfonic acid, 2-decyl-, compd. with 4-decylbenzenesulfonate, sodium salt (1:4:4)
CAS No.	22967-67-5
Synonyms	benzenesulfonic acid, o-decyl-, sodium salt, compd. with sodium p-decylbenzenesulfonate (1:4) benzenesulfonic acid, p-decyl-, sodium salt, compd. with sodium o-decylbenzenesulfonate (4:1)
Structural formula	
Molecular formula	$C_{16}H_{26}O_3S.{}^{1}/_{4}C_{16}H_{26}O_3S.{}^{5}/_{4}Na$

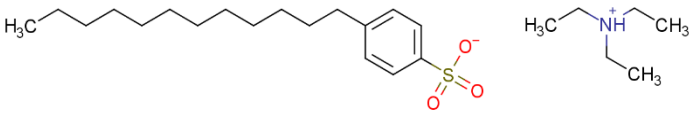
Molecular weight (g/mol)	1607.2
SMILES	[Na+].[Na+].CCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O.CCCCCCCCCCCC1=C(C=CC=C1)S([O-])(=O)=O
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1)
CAS No.	26264-05-1
Synonyms	isopropylamine dodecylbenzenesulfonate (INCI) dodecylbenzenesulfonic acid, monoisopropanolamine salt 2-propanamine, dodecylbenzenesulfonate
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_3H_9N$
Molecular weight (g/mol)	385.6
SMILES	CC(C)[NH3+].CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

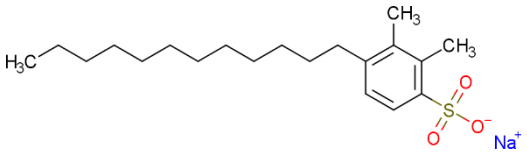
Chemical name	Benzenesulfonic acid, dodecyl-, compound with 2,2'-iminobis[ethanol] (1:1)
CAS No.	26545-53-9
Synonyms	DEA-dodecylbenzenesulfonate (INCI) diethanolamine, dodecylbenzene sulfonate
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_4H_{11}NO_2$
Molecular weight (g/mol)	431.6
SMILES	OCC[NH2+]CCO.CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

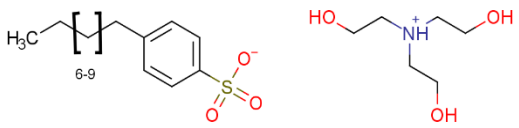
Chemical name	Benzenesulfonic acid, dodecyl-, compound with 2,2',2''-nitrilotris[ethanol] (1:1)

CAS No.	27323-41-7
Synonyms	TEA-dodecylbenzenesulfonate (INCI) dodecylbenzenesulfonic acid, triethanolamine salt ethanol, 2,2′,2″-nitrilotris-, dodecylbenzenesulfonate
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_6H_{15}NO_3$
Molecular weight (g/mol)	475.7
SMILES	OCC[NH+](CCO)CCO.CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

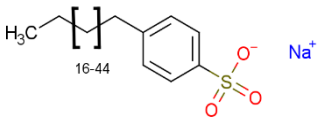
Chemical name	Benzenesulfonic acid, dodecyl-, compound with N,N-diethylethanamine (1:1)
CAS No.	29061-63-0
Synonyms	benzenesulfonic acid, dodecyl-, compound with triethylamine (1:1) triethylamine dodecylbenzenesulfonate (1:1) ethanamine, N,N-diethyl-, dodecylbenzenesulfonate
Structural formula	
Molecular formula	$C_{18}H_{30}O_3S.C_6H_{15}N$
Molecular weight (g/mol)	427.7
SMILES	CC[NH+](CC)CC.CCCCCCCCCCCCC1=CC=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

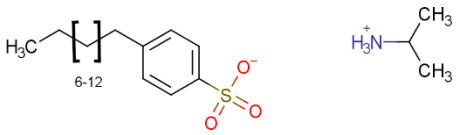
Chemical name	Benzenesulfonic acid, dodecyldimethyl-, sodium salt
CAS No.	63428-97-7
Synonyms	-

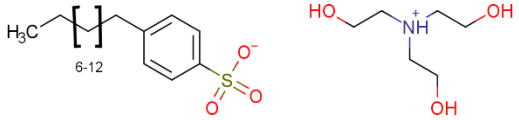
Structural formula	
Molecular formula	$C_{20}H_{34}O_3S.Na$
Molecular weight (g/mol)	376.5
SMILES	[Na+].CCCCCCCCCCCCC1=C(C)C(C)=C(C=C1)S([O-])(=O)=O
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, C10-13-alkyl derivatives, compounds with triethanolamine
CAS No.	68411-31-4
Synonyms	TEA-dodecylbenzenesulfonate (INCI) (C10-13) alkylbenzenesulfonic acid, triethanolamine salt
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, dodecyl-, branched
CAS No.	68411-32-5
Synonyms	(C12) branched alkylbenzenesulfonic acid
Structural formula	structure not available
Molecular formula	$C_{18}H_{30}O_3S$
Molecular weight (g/mol)	326.5
SMILES	unspecified
Chemical description	UVCB

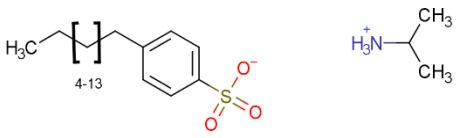
Chemical name	Benzenesulfonic acid, C20-48-alkyl derivatives, sodium salts
CAS No.	68555-09-9
Synonyms	linear C20-48-alkylbenzene bottoms, sulfonic acid, sodium salt
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with isopropylamine
CAS No.	68584-24-7
Synonyms	(C10-16) alkylbenzenesulfonic acid, isopropylamine salt
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

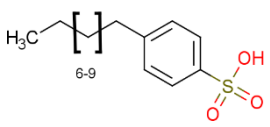
Chemical name	Benzenesulfonic acid, C10-16-alkyl derivatives, compounds with triethanolamine
CAS No.	68584-25-8
Synonyms	(C10-16) alkylbenzenesulfonic acid, triethanolamine salt
Structural formula	

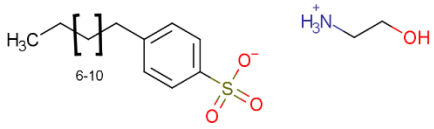
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, mono-C11-13-branched alkyl derivs., sodium salts
CAS No.	68608-89-9
Synonyms	-
Structural formula	structure not available
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

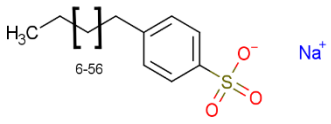
Chemical name	Benzenesulfonic acid, mono-C9-17-alkyl derivatives, compounds with isopropylamine
CAS No.	68953-93-5
Synonyms	(C9-17) branched alkylbenzenesulfonic acid, isopropylamine salt
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

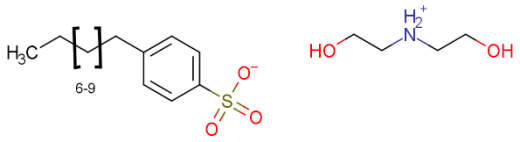
Chemical name	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives
CAS No.	85536-14-7

Synonyms	dodecylbenzene sulfonic acid (INCI)
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

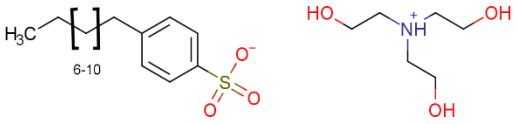
Chemical name	Benzenesulfonic acid, 4-C10-14-alkyl derivatives, compounds with ethanolamine
CAS No.	85995-82-0
Synonyms	benzenesulfonic acid, C10-14-alkyl derivatives, monoethanolamine salt
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, 2(or 4)-C10-14-alkyl derivatives, compounds with isopropanolamine
CAS No.	85995-83-1
Synonyms	benzenesulfonic acid, C10-14-alkyl derivatives, monoisopropanolamine salts
Structural formula	structure not available
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, C10-60-alkyl derivatives, sodium salts
CAS No.	90194-32-4
Synonyms	-
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with diethanolamine
CAS No.	90194-39-1
Synonyms	-
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, mono-C10-14-alkyl derivatives, compounds with triethanolamine
CAS No.	90194-42-6
Synonyms	TEA-dodecylbenzenesulfonate (INCI)

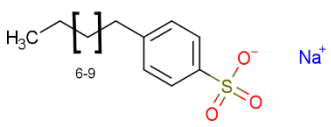
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

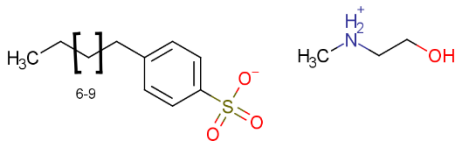
Chemical name	Benzenesulfonic acid, mono-C15-36-branched alkyl derivatives, sodium salts
CAS No.	90218-04-5
Synonyms	-
Structural formula	structure not available
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, 2,3(or 3,4)-dimethyl-, mono-C10-14-branched alkyl derivatives, sodium salts
CAS No.	90218-34-1
Synonyms	(C10-14) mixed branched alkyl o-xylene sulfonic acids, sodium salts
Structural formula	structure not available
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, methyl-, mono-C15-36-branched alkyl derivatives, sodium salts
CAS No.	90218-64-7

Synonyms	(C15-36) mixed branched alkyl toluene sulfonic acids, sodium salts
Structural formula	structure not available
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives, sodium salts
CAS No.	127184-52-5
Synonyms	-
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified
Chemical description	UVCB

Chemical name	Benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives, compounds with 2-(methylamino)ethanol
CAS No.	127620-18-2
Synonyms	-
Structural formula	
Molecular formula	unspecified
Molecular weight (g/mol)	unspecified
SMILES	unspecified

Chemical description	UVCB

Chemical name	Benzenesulfonic acid, (tetrapropenyl)-, compound with 2-propanamine (1:1)
CAS No.	157966-96-6
Synonyms	2-propanamine, (tetrapropenyl)benzenesulfonate
Structural formula	structure not available
Molecular formula	$C_{18}H_{28}O_3S.C_3H_9N$
Molecular weight (g/mol)	377.5
SMILES	unspecified
Chemical description	UVCB

Relevant physical and chemical properties

Pure ABS are solid at ambient temperatures. Based on the calculated vapour pressures <0.35 kPa at 20 ºC (calculated with EPI MPBPVP), chemicals in this group are expected to have low volatility. The melting point and the log K_{ow} (calculated with EPI WSKOW) increase with increasing alkyl chain length. The water solubilities of these chemicals are expected to be the highest for C10 with a critical micelle concentration (CMC) value of 0.1 g/L and lower with increasing chain length.

Introduction and use

Australia

There is currently no specific information about the introduction, use and end use of these chemicals in Australia.

International

The following international uses have been identified through the:

- Galleria Chemica
- European Union (EU) Registration, Evaluation and Authorisation of Chemicals (REACH) dossier
- Substances in Preparations in Nordic Countries (SPIN) database
- the European Cosmetic Ingredient Database (CosIng)
- United States Environmental Protection Agency (US EPA) Hazard Characterization Document
- Cosmetic Ingredient Review (CIR) report on dodecylbenzenesulfonate, decylbenzenesulfonate, and tridecylbenzenesulfonate salts

- Organisation for Economic Cooperation and Development (OECD) Screening Information Dataset (SIDS) Initial Assessment Report (SIAR) on Linear Alkylbenzene Sulfonate (LAS).

Seven chemicals (CAS Nos. 26264-05-1; 26545-53-9; 27323-41-7; 68411-31-4; 85536-14-7; 90194-39-1; 90194-42-6) have reported cosmetic uses as surfactants in cleansing and personal care products. TEA-dodecylbenzenesulfonate has reported use in hair styling hair care products (including shampoos and conditioners) and skin care products. The reported concentration range was 0.002–5% (CIR 2010).

All chemicals except CAS Nos. 3088-30-0; 11067-81-5 14356-38-8; 22967-67-5 63428-97-7 85995-82-0; 90218-64-7 and 127620-18-2 have reported domestic uses in:

- cleaning and washing agents (including stain remover, dishwasher detergent, dry cleaning kit for home use, car shampoo)
- colouring agents
- anti-static agents
- lubricants
- adhesive and binding agents.

Three chemicals (CAS Nos. 26264-05-1, 27323-41-7 and 26264-05-1) have reported uses in cleaning products at 5–10% (DeLima Associates). The Consumer Product Information Database (CPID) lists these chemicals in old products (toilet bowl cleaner/deodoriser and drain cleaner) at concentrations up to 30%.

The chemical CAS No. 26264-05-1 has reported use in an aerosol autocare product at <1%. Twelve chemicals (CAS Nos. 26264-05-1; 26545-53-9; 27323-41-7; 68411-31-4; 68411-32-5; 68584-24-7; 68584-25-8; 68608-89-9; 85536-14-7; 90194-32-4; 90218-04-5; 90218-34-1) have reported commercial uses in:

- industrial cleaning and foaming agents
- bleaching agents
- cutting fluids and lubricants
- adhesive and binding agents
- anti-freezing agents
- corrosion inhibitors
- surface treatment.

Based on the international use information, ABS are reported to be primarily used as surfactants in a wide range of domestic and commercial cleaning products and are listed on the US EPA High Production Volume (HPV) Challenge Program (US EPA 2014). LAS is reported to be present in laundry detergents and cleaners at concentrations up to 25 percent in consumer products, and up to 30 percent in commercial products (CIR 2010; OECD 2005). Concentrations up to 60% have been identified in liquid laundry capsules (NICNAS 2014a).

Four chemicals (CAS Nos. 26264-05-1; 68608-89-9; 85536-14-7; 90194-39-1) have reported site-limited uses in product formulation. ABSA in this group are typically intermediates in the production of ABS (US EPA 2004).

Several chemicals (CAS Nos. 12068-08-5; 26264-05-1; 27323-41-7; 29061-63-0; 68411-31-4; 68411-32-5; 68584-24-7; 68584-25-8; 68953-93-5; 85536-14-7; 90194-39-1; 90194-42-6; 127184-52-5; 157966-96-6) have reported non-industrial uses in agricultural pesticides.

Existing Australian regulatory controls

AICIS

No specific controls are currently available for these chemicals.

Public

No specific controls are currently available for these chemicals.

Following concerns relating to child exposure to the contents of liquid laundry capsules, the ACCC jointly established with industry an Australian Industry Guideline for Labelling & Packaging of Liquid Laundry Capsules (ACCC 2015).

Workers

These chemicals are not listed on the Hazardous Chemical Information System (HCIS) (Safe Work Australia, SWA).

No exposure standards are available for these chemicals in Australia (SWA).

International regulatory status

Exposure standards

The following exposure standards were identified (Chemwatch):

Time weighted average (TWA): 2 mg/m^3 — Japan, United States of America (CAS Nos. 26545-53-9; 27323-41-7; 68411-31-4; 68584-24-7; 68584-25-8; 68953-93-5; 90194-32-4; 90194-42-6)

TWA: 2 mg/m^3 — Japan (CAS Nos. 68555-09-9; 90194-39-1; 90218-04-5)

TWA: 2 mg/m^3 — United States of America (CAS Nos. 26264-05-1; 85995-82-0; 127184-52-5)

Health hazard information

Toxicokinetics

No toxicokinetic data are available for this group of chemicals.

In general, LAS are readily absorbed through the gastrointestinal tract, are distributed throughout the body and are extensively metabolised. The parent compound and metabolites are excreted primarily in the urine and faeces. However, the main route of excretion is isomer dependent. The limited evidence available shows that dermal absorption of LAS is low, although prolonged contact may compromise the dermal barrier and allow increased absorption to occur (HERA 2013).

Acute toxicity

Oral

Based on the available data, chemicals in this group are considered to have moderate acute toxicity following oral exposure.

In a GLP compliant acute oral toxicity study conducted in accordance with OECD Test Guideline (TG) 423, 6 female Wistar rats were treated with a single dose of 2000 mg/kg bw of benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1). The reported median lethal dose (LD50) was >2000 mg/kg bw. Reported clinical signs of toxicity included hunched posture, piloerection and salivation (REACHa).

In a GLP compliant acute oral toxicity study conducted in accordance with OECD TG 401, Wistar rats (5/sex/dose) were treated with 1250, 1415, 1580 or 1990 mg/kg bw of benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7). The calculated LD50 value was 1470 mg/kg bw. Reported clinical signs of toxicity included dry skin, diarrhoea, squatting attitude, small dark red eyes, ataxia, hypothermia, diuresis, occasional trembling, tumbling, and prone position (REACHb).

In two non-GLP compliant acute oral toxicity studies conducted in accordance with OECD TG 401, rats (strains not identified) (5/sex/dose) were treated with single doses of 200–3200 mg/kg bw of benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with diethanolamine (CAS No. 90194-39-1). The reported LD50 values were 1080 and 1600 mg/kg bw. Reported clinical signs of toxicity included diarrhoea, dyspnoea, scrubby coat nose bleeding, ataxia, and lethargy (REACHc).

The following median lethal dose (LD50) values in rats were reported:

- 1000 mg/kg bw for benzenesulfonic acid, tetrapropylene- (CAS No. 11067-81-5) (CCOHS 1974)
- 1300 mg/kg bw for benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) (US EPA 2014)
- 1653 and >1953 mg/kg bw for benzenesulfonic acid, dodecyl-, compound with 2,2',2''-nitrilotris[ethanol] (1:1) (CAS No. 27323-41-7) (CCOHS 2002; US EPA 2014)
- 1080–1260 mg/kg bw for benzenesulfonic acid, dodecyl-, branched (CAS No. 68411-32-5) (CCOHS 2002; US EPA 2014)
- 1200 mg/kg bw for benzenesulfonic acid, C10-16-alkyl derivatives, compounds with triethanolamine (CAS No. 68584-25-8) (Chemwatch)
- 1200 mg/kg bw for benzenesulfonic acid, mono-C10-14-alkyl derivatives, compounds with triethanolamine (CAS No. 90194-42-6) (Chemwatch)
- 438 mg/kg bw for benzenesulfonic acid, 2,3(or 3,4)-dimethyl-, mono-C10-14-branched alkyl derivatives, sodium salts (CAS No. 90218-34-1) (Chemwatch)

Other LASs were reported to have moderate acute toxicity via the oral route in rats and mice with LD50 values in the ranges of 404–1470 mg/kg bw in rats and 1250–2300 mg/kg bw in mice. Reported signs of toxicity include piloerection, diarrhoea, weakness and changes in motor activity. Convulsions, torsion and paralysis of the hind limbs were also observed in mice (NICNAS 2014a).

Dermal

Based on the limited data available these chemicals do not warrant hazard classification. Whilst several unreliable studies indicating moderate dermal toxicity are available for the analogue chemicals (LASs) (NICNAS 2014a), the available studies indicate low dermal toxicity.

In a GLP compliant acute dermal toxicity study conducted in accordance with OECD TG 402, CFY rats (5/sex/dose) were treated with a single dose of 2000 mg/kg bw of benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with diethanolamine (CAS No. 90194-39-1). The reported dermal LD50 value was >2000 mg/kg bw. Slight erythema and oedema of treated skin was reported (REACHc).

The reported LD50 in rabbits is >4199 mg/kg bw for benzenesulfonic acid, dodecyl-, compound with 2,2',2''-nitrilotris[ethanol] (1:1) (CAS No. 27323-41-7) (CCOHS 2002; US EPA 2014).

Inhalation

No data are available for chemicals in this group.

In a study reported in HERA (2013), LAS (C12) caused acute effects in an animal test following inhalation exposure. Rats (8/dose) underwent nose-only exposure to aerosol atmospheres (with a mean mass aerodynamic diameter of 2.5 µm) of the chemical at concentrations of 0.065, 0.12, 0.26 and 0.31 mg/L for 4 h. No mortalities or adverse clinical signs were reported up to a concentration of 0.26 mg/L. At the highest dose there were three mortalities. The median lethal concentration (LC50) was not determined. Observed sub-lethal effects included clear to red nasal discharge.

Corrosion/Irritation

Corrosion

Based on the available data for benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) and other LASA, ABSA in this group (CAS Nos. 85536-14-7; 11067-81-5; 68411-32-5) are expected to be corrosive to skin. Corrosive chemicals are also considered to cause irreversible effects in the eyes.

In a skin irritation study conducted in accordance with OECD TG 404, New Zealand White (NZW) rabbits (3/sex) were treated with benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) for 4 hours under occluded conditions. Observations were recorded at 1, 24, 48 and 72 hours, and at 6, 9 and 14 days after patch removal. The following mean scores were reported for observations at 24, 48 and 72 hours: 4, 4, 4 for erythema and 1, 1, 2 for oedema respectively (maximum score 0 of 4). The erythema and oedema were not reversible in any of the animals within 14 days (REACHb).

Application of 0.5 mL of benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) to the skin of rabbits resulted in severe irritation (CCOHS 2003). No further details are available.

Undiluted benzenesulfonic acid, dodecyl-, branched (CAS No. 68411-32-5) (0.5 g; 93–95% purity) was applied to intact skin of 3 NZW rabbits (sex not specified) under occluded

conditions for 4 hours. The animals were observed for up to 72 hours. The chemical was irritating to skin (US EPA 2014). No further details are available.

LASAs are strongly acidic with a pH <2 and therefore it can be predicted that, when applied to healthy intact skin, full thickness destruction of the skin tissue is possible. Chemical burns and necrosis have been observed in an animal study (NICNAS 2014b).

Skin irritation

Based on the weight of evidence of available data for these chemicals and structurally similar chemicals, ABS in this group are considered to be skin irritants.

In a GLP compliant in vitro skin irritation study conducted in accordance with OECD TG 439 (in vitro reconstructed human epidermis (RhE) test method for skin irritation), benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) was applied to RhE for an exposure period of 15 (± 0.5) minutes, followed by an observation period of 42 hours. The mean tissue viability was 22%. Irritant chemicals are identified by their ability to decrease cell viability below the defined threshold level ≤50%. Therefore, the chemical is considered to be a skin irritant. Interpretation of results obtained from OECD TG 439 studies do not allow for distinction between irritation and corrosion (REACHa).

In a GLP compliant in vitro skin corrosion assay conducted in accordance with OECD TG 431, benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) was applied to reconstructed human epidermis EpiDERM™ for 3 and 60 minutes. The mean tissue viability was 93% and 78% after 3 and 60 minutes, respectively. Only chemicals that reduce viability to less than 50% and 15% after 3 and 60 minutes are classified as corrosive. Therefore, the chemical is unlikely to be corrosive following in vivo application (REACHa).

Undiluted benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) (0.5 mL; 90.9% purity) was applied to intact and abraded skin of 6 NZW rabbits (sex not specified) under semi-occluded conditions for 24 hours. The animals were observed for up to 72 hours. The chemical was irritating to skin (US EPA 2014). No further details are available.

Undiluted benzenesulfonic acid, dodecyl-, compound with 2,2',2''-nitrilotris[ethanol] (1:1) (CAS No. 27323-41-7) (0.5 g; 60% purity) was applied to intact skin of 3 NZW rabbits (sex not specified) under occluded conditions for 4 hours. The animals were observed for up to 72 hours. The chemical was irritating to skin (US EPA 2014). No further details are available.

Several guideline studies conducted in rabbits for structurally similar LAS showed irritation effects. No irritation effects were observed in rabbits at concentrations of 1–2.5%. LAS is moderately irritating at 5% and severely irritating to skin at concentrations above 15% (CIR 2010; HERA 2013; NICNAS 2014a; OECD 2005; US EPA 2014).

Eye irritation

Limited data are available. Based on the weight of evidence across this group of chemicals and structurally similar LAS, these chemicals should be classified for serious eye damage unless data for individual chemicals are available to indicate otherwise.

In a GLP compliant ex vivo eye corrosivity/irritation study conducted according to OECD TG 437, benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-

05-1) was applied to 3 bovine cornea per experiment. The mean in vitro irritancy score (IVIS) was 11 (IVIS >55 is regarded as serious eye damage and IVIS ≤3 is UN GHS No Category). Based on the criteria of the assay, no stand-alone prediction can be made. The chemical does not meet the GHS criteria for serious eye damage classification (REACHa). Although the concentration used in this study was not reported, surfactant substances are typically tested at a concentration of 10% w/v according to the OECD test guideline.

In a GLP compliant in vitro eye corrosion study conducted according to OECD TG 492, benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) (50 µL, undiluted) was topically applied to reconstructed human cornea-like epithelium (RhCE) using the EpiOcular™ EIT test method for the liquids protocol and tissue viability was measured following exposure and a post-treatment incubation period. The tissue viability was determined to be 12. Based on the decision criteria for this test (tissue viability >60% for EpiOcular™ EIT liquids' protocol), no prediction can be made. The chemical does not meet the criteria for not requiring classification (REACHa). Although the concentration used in this study was not reported, surfactant substances are typically tested at a concentration of 10% w/v according to the OECD test guideline.

Undiluted benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) (0.1 mL; 90.9% purity) was applied to the eyes of NZW rabbits (sex not specified). Observations were recorded at 24, 48, 72 hours, and at 4 and days. The chemical was irritating to the eye (US EPA 2014). No further details are available.

Application of 0.1 mL of benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) to the eye of rabbits resulted in severe irritation (CCOHS 2002). No further details are available.

In a non-GLP compliant eye irritation study conducted in accordance with OECD TG 405, 0.1 mL of benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) was instilled into the conjunctival sac of one eye each of NZW rabbits (3/sex). Observations were recorded at 1, 24, 48, 72 hours, and at 6 days. The following mean scores were reported at 24, 48 and 72 hours: corneal opacity (3.66/4, 3.66/4, 3.33/4), iritis (1/2, 1/2, 1/2), conjunctival redness (3/3, 3/3, 3/3), and chemosis (2/4, 2/4, 2/4). The observed effects were not reversible in any of the animals within 6 days (REACHb).

Application of 0.1 mL of benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) to the eye of rabbits resulted in moderate irritation (CCOHS 2003). No further details are available.

Several guideline studies in rabbits showed that structurally similar LAS were not irritating to the eye at concentrations up to 1%, moderately irritating at 5% and severely irritating at 47–50% (HERA 2013; NICNAS 2014a; OECD 2005; US EPA 2014).

Sensitisation

Skin sensitisation

While in vitro and in silico studies suggest that some chemicals in this group may have skin sensitisation potential, based on the weight of evidence of data for chemicals across this group and structurally similar LAS and LASA (HERA 2013; NICNAS 2014b; OECD 2005), chemicals in this group are unlikely to be potent skin sensitisers.

In a GLP compliant in vitro skin sensitisation study conducted in accordance with OECD TG 442C (direct peptide reactivity assay (DPRA)), benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) dissolved in acetonitrile/water (1:1, v/v) was reported positive using defined ratios of peptide to test item (1:10 cysteine peptide, 1:50 lysine peptide). Mean cysteine and lysine depletion by the chemical was 42.6%, indicating peptide binding (REACHa).

In a GLP compliant in vitro keratinocyte activation test (LuSens assay) conducted in accordance with OECD TG 442D, benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) was reported to be positive (activation of the antioxidant/electrophile responsive element (ARE)-dependent pathway in keratinocytes) up to a concentration of 31 µM. The chemical induced a significant luciferase activity as fold induction remained >1.5, indicating keratinocyte activation (REACHa).

In an in vivo skin sensitisation study described as being a guinea pig maximisation test (GPMT), intradermal induction was performed using benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) at 0.05% in corn oil with adjuvant and topical induction with the chemical at 5% in corn oil. The animals were also challenged with the chemical at 2.5% in corn oil. None of the treated animals showed skin reactions. The chemical was reported to be non-sensitising in this study (REACHb).

In a GLP-compliant GPMT (reported as a read across source, unknown constituents) conducted in accordance with OECD TG 406, intradermal induction was performed on Hartley guinea pigs (10/sex) using 25% benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with diethanolamine (CAS No. 90194-39-1) in water and topical induction with the chemical at 25% in water. Challenge with the chemical at 12.5% in water resulted in no skin reactions (REACHc).

Several studies in guinea pigs showed no sensitisation effect for LAS and LASA at concentrations up to 50% (HERA 2013; NICNAS 2014b; OECD 2005).

Observation in humans

There was no evidence of skin sensitisation for LAS at concentrations of 0.1% and 1% in human repeated patch tests (HRIPT) and exposure studies (HERA 2013; OECD 2005).

In silico data

The knowledge based expert system Deductive Estimation of Risk from Existing Knowledge (DEREK) Nexus version 6.0.1 was utilised to estimate the skin sensitisation potential of this group of chemicals. An alert for skin sensitisation by alkyl sulfate or sulfonate was reported for one chemical. It is likely to interact with skin proteins by nucleophilic substitution on sulfonates. The predicted effective concentration for a 3 fold increase in lymphocyte proliferation in local lymph node assay (LLNA EC3) for benzenesulfonic acid, tetrapropylene- (CAS No. 11067-81-5) was 4.3% indicating moderate sensitisation potential.

Repeat dose toxicity

Oral

No data are available. Based on the available data for previously assessed structurally similar LAS and LASA (HERA 2013; NICNAS 2014b; OECD 2005; US EPA 2014), chemicals

in this group are not likely to cause serious damage to health following repeated oral exposure.

In several repeated dose studies ranging between 28 days and 2 years in rats and mice treated with LAS via gavage, in feed and drinking water, the no observed adverse effect levels (NOAELs) ranged from 40 to 250 mg/kg bw/day. Reported adverse effects include reduced body weight gain, diarrhoea, increases in relative liver weight, differences in enzymatic and serum-biochemical parameters, and mild degeneration and desquamation of the tubular epithelium in the kidneys (HERA 2013; NICNAS 2014a; OECD 2005; US EPA 2014).

In a 28 day study in rats with a structurally similar LASA local effects at the site of contact (stomach) were observed (NICNAS 2014b).

Dermal

Based on the available data for benzenesulfonic acid, mono-C15-36-branched alkyl derivatives, sodium salts (CAS No. 90218-04-5) and data for structurally similar chemicals, chemicals in this group (HERA 2013; NICNAS 2014a; OECD 2005; US EPA 2014) are not likely to cause serious damage to health following repeated dermal exposure. However, chemicals in this group may compromise the integrity of the skin and increase dermal absorption of other chemicals present product formulations.

In a non-guideline 28-day repeated dose toxicity study conducted similar to OECD TG 410, NZW rabbits (10/sex/dose) were administered benzenesulfonic acid, mono-C15-36-branched alkyl derivatives, sodium salts (CAS No. 90218-04-5) by dermal application at 2 mL/kg of 5 or 25% (w/w) concentrations for 24 h/day, 5 days/week for 4 weeks. No mortality was reported. An increase in relative brain and adrenal weights were reported in females at the high dose group. The no observed adverse effect level (NOAEL) was determined to be 2 mL/kg bw of 5% (w/w) concentration (ChemWatch). No further details are available for the study.

In a study reported in OECD SIDS (2005), male Wistar rats were treated with LAS dosage equivalent of 286 and 427 mg/kg bw/day for 15 days. Body weight gain was reduced in the low dose group and body weight decreased in the high dose group. Severe necrosis and severe infiltration of leukocytes at the application site were observed in both groups at 4–6 days and continued during the study. No other systemic effects were observed. Effects were attributed to local irritant effects.

Structurally similar LAS produced no treatment-related systemic effects in repeated dose dermal toxicity studies in rats although skin corrosion effects were observed.

Inhalation

No data are available for chemicals in this group or structurally similar LAS or LASA.

Genotoxicity

Based on the available data and data for structurally similar LAS and LASA (HERA 2013; NICNAS 2014a; NICNAS 2014b; OECD 2005; US EPA 2014), chemicals in this group are not expected to be genotoxic.

In vitro

Negative results were reported for benzenesulfonic acid, dodecyl-, compound with 2-propanamine (1:1) (CAS No. 26264-05-1) in a bacterial reverse mutation assay (OECD TG 471) in *Salmonella typhimurium* strains TA 98, TA 100, TA 1535 and TA 1537, and *Escherichia coli* WP2 uvrA with and without metabolic activation (S9) at concentrations up to 2500 µg/plate (REACHa).

Negative results were reported in the following in vitro genotoxicity studies (reported as read-across source, unknown constituents) for benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with diethanolamine (CAS No. 90194-39-1) (REACHc):

- two bacterial reverse mutation assays (OECD TG 471) in *S. typhimurium strains* TA 1535, TA 1537, TA 1538, TA 98 and TA100, and *E. coli* WP2 and WP2uvrA with and without metabolic activation (S9) at concentrations up to 4000 µg/plate
- a chromosome aberration study (OECD TG 473) in Chinese hamster ovary (CHO) cells with and without metabolic activation at concentrations up to 3010 µg/mL
- two mammalian cell gene mutation studies (OECD TG 476) in CHO cells at concentrations up to 100 µg/mL or the thymidine kinase (TK) locus in mouse lymphoma L5178Y cells at concentrations up to 400 µg/mL with and without metabolic activation
- a sister chromatid exchange (SEC) assay (OECD TG 479) in CHO cells with and without metabolic activation at concentrations up to 1500 µg/mL.

Negative results were reported for LAS and LASA in several in vitro bacterial reverse mutation assays in *S. typhimurium* strains TA 98, TA 100, TA 1535, TA 1537 and TA 1538 with and without metabolic activation (S9) at concentrations up to 5000 µg/plate. Negative results were also reported in a recombination assay using *Bacillus subtilis* at concentrations up to 50 µg/plate and in an *E. coli* (WP2uvrA) reverse mutation assay with and without activation (HERA 2013; NICNAS 2014a; NICNAS 2014b; OECD 2005; US EPA 2014). Similarly negative results were observed for LAS in three mammalian cell mutation studies at concentrations below cytotoxicity level (HERA 2013).

In vivo

In a GLP compliant mammalian erythrocyte micronucleus test conducted similar to OECD TG 474, NMRI mice (40/sex) were administered benzenesulfonic acid, 4-C10-13-sec-alkyl derivatives (CAS No. 85536-14-7) as a single dose at 1122 mg/kg bw by gavage. There were no significant increases in the incidence of micronuclei in polychromatic erythrocytes, indicating a lack of clastogenicity (REACHb).

Chemicals LAS or LASA did not induce clastogenic effects in cytogenetic assays in rats and mice, in a dominant lethal assay in rats, and in a micronucleus test in mice (HERA 2013; NICNAS 2014a; NICNAS 2014b; OECD 2005; US EPA 2014).

Carcinogenicity

No data are available. Structurally similar LAS were not reported to be carcinogenic in 2-year carcinogenicity studies in rats (HERA 2013; OECD 2005; US EPA 2014). Therefore, chemicals in this group are not expected to have carcinogenic potential.

In four 2-year carcinogenicity studies, LAS was administered to rats at concentrations up to 300 mg/kg bw/day in diet or 200 mg/kg bw/day in drinking water. No gross or

histopathological evidence of tumorigenesis or carcinogenic effect were reported in these studies (HERA 2013; NICNAS 2014a; OECD 2005; US EPA 2014).

Reproductive and development toxicity

No data are available for chemicals in this group. Structurally similar LAS showed no evidence of reproductive and developmental toxicity in rats, mice and rabbits (HERA 2013; OECD 2005). Therefore, chemicals in this group are not expected to cause specific adverse effects on fertility, sexual function or development following oral and dermal exposure.

In three reproductive studies, LAS was administered to rats in feed for three to four generations. There was no evidence of reproductive, fertility or developmental toxicity effects reported in these studies. The reported NOAEL values were 70–350 mg/kg bw/day for reproductive and developmental toxicity (HERA 2013; OECD 2005).

In 17 developmental and teratogenicity toxicity studies, LAS was administered to rats, mice and rabbits via oral (gavage, in feed or drinking water) or dermal routes at concentrations up to 600 and 1500 mg/kg bw/day, respectively. Adverse developmental effects including embryo death or deformities and litter loss were reported at maternally toxic doses associated with the irritation effects of LAS (either on the skin or the gastrointestinal tract). No decreases in litter size, malformations or significant skeletal defects were observed compared to controls in rats (orally up to 780 mg/kg bw/day), mice (dermally up to 500 mg/kg bw/day) and rabbits (dermally up to 90 mg/kg bw/day) (HERA 2013; NICNAS 2014a; OECD 2005).

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