Linear alkylbenzenesulfonates (C10-C16): Human health tier II assessment

07 February 2014

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Chemicals in this assessment

Chemical Name in the Inventory	CAS Number
Benzenesulfonic acid, decyl-, sodium salt	1322-98-1
Benzenesulfonic acid, dodecyl-, ammonium salt	1331-61-9
Benzenesulfonic acid, 4-dodecyl-, sodium salt	2211-98-5
Benzenesulfonic acid, dodecyl-, sodium salt	25155-30-0
Benzenesulfonic acid, dodecyl-, compound with 2-aminoethanol (1:1)	26836-07-7
Benzenesulfonic acid, dodecyl-, potassium salt	27177-77-1
Benzenesulfonic acid, 4-dodecyl-, compound with 2-aminoethanol (1:1)	58089-99-9
Benzenesulfonic acid, mono-C10-16-alkyl derivatives, sodium salts	68081-81-2
Benzenesulfonic acid, C10-13-alkyl derivatives, sodium salts	68411-30-3

Chemical Name in the Inventory	CAS Number
Benzenesulfonic acid, dodecyl-, reaction products with ethanolamine	68442-72-8
Benzenesulfonic acid, C10-16-alkyl derivatives, potassium salts	68584-27-0
Benzenesulfonic acid, mono-C10-16-alkyl derivatives, ammonium salts	68910-31-6
Benzenesulfonic acid, mono-C10-16-alkyl derivatives, compounds with 2-aminoethanol	68910-32-7
Benzenesulfonic acid, C10-14-alkyl derivatives, sodium salts	69669-44-9
Benzenesulfonic acid, mono-C10-13-alkyl derivatives, ammonium salts	85480-54-2
Benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with ethanolamine	85480-55-3
Benzenesulfonic acid, mono-C10-13-alkyl derivatives, potassium salts	85480-57-5
Benzenesulfonic acid, 4-C10-14-alkyl derivatives, sodium salts	91696-66-1

Preface

This assessment was carried out by staff of the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) using the Inventory Multi-tiered Assessment and Prioritisation (IMAP) framework.

The IMAP framework addresses the human health and environmental impacts of previously unassessed industrial chemicals listed on the Australian Inventory of Chemical Substances (the Inventory).

The framework was developed with significant input from stakeholders and provides a more rapid, flexible and transparent approach for the assessment of chemicals listed on the Inventory.

Stage One of the implementation of this framework, which lasted four years from 1 July 2012, examined 3000 chemicals meeting characteristics identified by stakeholders as needing priority assessment. This included chemicals for which NICNAS already held exposure information, chemicals identified as a concern or for which regulatory action had been taken overseas, and chemicals detected in international studies analysing chemicals present in babies' umbilical cord blood.

Stage Two of IMAP began in July 2016. We are continuing to assess chemicals on the Inventory, including chemicals identified as a concern for which action has been taken overseas and chemicals that can be rapidly identified and assessed by using Stage One information. We are also continuing to publish information for chemicals on the Inventory that pose a low risk to human health or the environment or both. This work provides efficiencies and enables us to identify higher risk chemicals requiring assessment.

The IMAP framework is a science and risk-based model designed to align the assessment effort with the human health and environmental impacts of chemicals. It has three tiers of assessment, with the assessment effort increasing with each tier. The

Tier I assessment is a high throughput approach using tabulated electronic data. The Tier II assessment is an evaluation of risk on a substance-by-substance or chemical category-by-category basis. Tier III assessments are conducted to address specific concerns that could not be resolved during the Tier II assessment.

These assessments are carried out by staff employed by the Australian Government Department of Health and the Australian Government Department of the Environment and Energy. The human health and environment risk assessments are conducted and published separately, using information available at the time, and may be undertaken at different tiers.

This chemical or group of chemicals are being assessed at Tier II because the Tier I assessment indicated that it needed further investigation.

For more detail on this program please visit:**www.nicnas.gov.au**

Disclaimer

ACRONYMS & ABBREVIATIONS

Grouping Rationale

The chemicals in this group are salts of structurally related linear alkylbenzene sulfonates (LASs) that have surfactant properties.

The chemicals in this group can have an alkyl chain between 10 and 16 carbon atoms. The main commercial grade material is typically limited to a range of 10–14 or 10–13 carbons with a dodecyl-component of 20–35 %. The carbon chain distribution of the chemicals will vary depending on the method of production and the source of the precursor chemicals. The average molecular weight of the anion is expected to be similar to that of sodium dodecylbenzene sulfonate (CAS No. 25155-30-0).

The chemicals are usually a mixture of homologues and phenyl positional isomers, each containing a sulfonated aromatic ring and a linear alkyl chain attached at any position except for the sulfonated carbon (IPCS 1996). The proportions are determined by the starting materials. They are manufactured by reacting the parent alkylbenzenes with sulfuric acid or sulfur trioxide to give the corresponding sulfonic acid which is neutralised to the desired salt; usually sodium but may include ammonium, potassium and monoethanolamine (the chemicals in this group) and calcium and magnesium. This would be expected to give mostly 2- and 4-substitution, with a steric preference for 4.

The solubility of the homologues differs based on the alkyl chain length, usually decreasing with increasing chain length. However, as the chemicals are also mixtures of positional isomers, chemicals with the same alkyl chain distribution (same average carbon number) can have different properties depending on the 2-phenyl isomer content (consistent with 4-substitution as the major product with smaller amounts of the 2-substitution) (IPCS 1996).

Most of the chemicals in this group have similar end uses, typically in cleaning products. The chemicals in this group are expected to have similar toxicity, which is primarily due to the alkylbenzene sulfonate anion. They share similar physico-chemical properties, including density and melting points.

Import, Manufacture and Use

Australian

The following Australian industrial uses were reported under previous mandatory and/or voluntary calls for information:

The following chemicals have reported domestic use as surfactants in cleaning and washing agents:

- sodium dodecylbenzene sulfonate (CAS No. 25155-30-0)
- sodium mono-(C10-16)-alkylbenzene sulfonate (CAS No. 68081-81-2)
- sodium mono-(C10-14)-alkylbenzene sulfonate (CAS No. 69669-44-9)

Monoethanolamine dodecylbenzenesulfonate (CAS No. 26836-07-7) has been identified in cleaning and washing agents up to 60 % concentration.

International

The following international uses have been identified through European Union Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) dossiers; the Organisation for Economic Cooperation and Development Screening Information Data Set International Assessment Report (OECD SIAR); Galleria Chemica; Substances and Preparations in the Nordic countries (SPIN) database; the European Commission Cosmetic Ingredients and Substances (CosIng) database; United States (US) Personal Care Product Council International Nomenclature of Cosmetic Ingredients (INCI) Dictionary; American Cleaning Institute (ACI) Cleaning product ingredient inventory; and eChemPortal: OECD High Production Volume chemical program—OECD HPV, the US Environmental Protection Agency's Aggregated Computer Toxicology Resource—ACToR, and the US National Library of Medicine's Hazardous Substances Data Bank—HSDB.

The chemicals (CAS Nos 1322-98-1, 1331-61-9, 25155-30-0, 27177-77-1 and 26836-07-7) are reported in the CosIng database with the identified cosmetic functions of cleansing and emulsifying.

LASs are an important group of synthetic anionic surfactants in widespread use in laundry detergents and cleaning agents with 78-97 % of worldwide consumption of these chemicals in this product category (OECD SIDS 2005). All the chemicals have reported domestic use including:

- as a surfactant; and
- cleaning and washing agents.

The chemicals (CAS Nos 1331-61-9, 25155-30-0 and 68411-30-3) have reported domestic use in paints, lacquers and varnishes.

The chemicals (CAS Nos 25155-30-0 and 68411-30-3) have reported domestic use including in:

- adhesives and binding agents;
- colouring agents;
- corrosion inhibitors; and
- surface treatment.

The chemicals (CAS Nos 25155-30-0 and 68411-30-3) have reported site-limited use as electroplating agents.

The chemicals (CAS Nos 25155-30-0 and 68411-30-3) have reported non-industrial use including:

- non-agricultural pesticides and preservatives; and
- agricultural pesticides.

The following chemicals have no identified uses internationally; this does not preclude future use in products in the same categories as identified above:

- sodium 4-dodecylbenzenesulfonate (CAS No. 2211-98-5);
- monoethanolamine 4-dodecylbenzene sulfonate (CAS No. 58089-99-9);

- 4-dodecylbenzenesulfonic acid, monoethanolamine salt (CAS No. 68442-72-8);
- ammonium mono-(C10-13)-alkylbenzenesulfonate (CAS No. 85480-54-2); and
- sodium 4-(C10-14)-alkylbenzenesulfonate (CAS No. 91696-66-1).

Restrictions

Australian

Sodium dodecylbenzene sulfonate (CAS No. 25155-30-0) is listed in the Poisons Standard (Standard for the Uniform Scheduling of Medicines and Poisons 2013—SUSMP) in Schedule 5 except for preparations containing 30 per cent or less of sodium dodecylbenzene sulfonate.

International

The following regulation applies to the monoethanolamine salts of LAS (CAS Nos 26836-07-7, 58089-99-9, 68442-72-8, 68910-32-7 and 85480-55-3):

EU Cosmetics Regulation 1223/2009 Annex III—List of substances which cosmetic products must not contain except subject to the restrictions laid down;

Monalkylamines, monoalkanolamines and their salts.

- maximum secondary amine content in the finished product: 0.5 %.
- minimum raw material purity: 99 %.
- maximum secondary amine content in the raw materials: 0.5 % (applies).
- maximum nitrosamine content 50 µg/kg.
- should not be used with nitrosating systems and should be kept in nitrite-free environments.

Existing Worker Health and Safety Controls

Hazard Classification

Sodium dodecylbenzene sulfonate (CAS No. 25155-30-0) is classified as hazardous, with the following risk phrases for human health in the Hazardous Substances Information System (HSIS) (Safe Work Australia):

Xn; R22: Harmful if swallowed

Exposure Standards

Australian

No specific exposure standards are available.

International

No specific exposure standards are available.

Health Hazard Information

The cation components of the chemicals (that is sodium, potassium, ammonium and monoethanolamine) are not expected to contribute significantly to the toxicity of the chemicals. In studies where the chemical was not identified by CAS No., the generic term linear alkylbenzene sulfonate (LAS) will be used, and is usually in the form of the sodium salt. Where stated, the numbers following 'C' indicate the range of carbon chain units.

Toxicokinetics

LASs 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 salts is low, although prolonged contact may compromise the dermal barrier and allow increased absorption to occur (IPCS 1996; HERA 2013).

Oral administration of sodium salts of LAS (C12) to Wistar rats showed rapid distribution to stomach, intestines, urinary bladder, liver, kidney, testis, spleen and lung. After 168 hours, 47–50 % of the salts were excreted in urine and 50–51 % in the faeces. Oral administration of LAS (C12) with various 2- and 4-substitution ratios showed marked differences in excretion. The 2-isomer was mainly excreted in urine (75 %) but the 4-isomer was mainly excreted in the faeces (77.9 %).

Sodium dodecylbenzene sulfonate (CAS No. 25155-30-0) was fed in the diet daily to male rats for five weeks. During the dosing period 81.8 % was excreted with 52.4 % in the faeces and 29.4 % in urine. After a further week on a normal diet 7.8 % of estimated residual chemical was found in excreta.

In an implantation disturbance study, LAS was not detected in the reproductive organs (uterus and ovaries) of pregnant ICR mice administered a single oral dose of 350 mg/kg bw on day 3 of gestation.

Acute Toxicity

Oral

Sodium dodecylbenzene sulfonate (CAS No. 25155-30-0) is classified as hazardous with the risk phrase ‘Harmful if swallowed’ (Xn; R22) in HSIS (Safe Work Australia). There are numerous study data available for sodium salts of LAS with a carbon range of C9-15 (IPCS 1996; HERA 2013). The median lethal dose (LD50) of 404–1470 mg/kg bw in rats and 1250–2300 mg/kg bw in mice support this classification for all the chemicals in this group. 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.

In numerous studies reported in OECD SIDS (2005) a higher range of LD50s were reported; the LD50 values were 1080–1980 mg/kg bw in rats and 2160 and 2250 mg/kg bw for male and female mice, respectively. The LD50 values for rats support classification of the chemicals in this group.

Dermal

Sodium (C10-13)-alkylbenzene sulfonate (CAS No. 68411-30-0) had low acute toxicity in an animal test (to OECD Test Guideline (TG) 402) following dermal exposure. The LD50 in rats is greater than 2000 mg/kg bw. Well-defined or slight erythema and slight oedema were observed after removal of the occlusive dressing (REACH a,b; HERA 2013).

There were several unreliable studies reported in OECD SIDS (2005) with LD50s ranging from >631 mg/kg bw to <1000 mg/kg bw in rabbits. Adverse effects included lung hyperaemia, liver discolouration and gastrointestinal inflammation. However, in these

studies, the concentration of sodium LAS was not reported and there was an insufficient number of animals (one per dose) (OECD SIDS 2005).

Inhalation

Based on the data available, the chemicals in this group may be toxic by inhalation. However, the data available are not sufficient to allow hazard classification.

In a study reported in HERA (2013), LAS (C12) caused acute effects in an animal test following inhalation exposure. Rats (eight per group) 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

Respiratory Irritation

Based on the effects reported in skin and eye irritation tests and the acute inhalation toxicity study, high concentrations of the chemicals are likely to be irritating if significant exposure to aerosols occurs.

Skin Irritation

Numerous skin irritation studies were reported in HERA (2013), REACH (a,b), IPCS (1996) and OECD SIDS (2005) which support the classification of the chemicals in this group as skin irritants.

One study was performed in accordance with OECD TG 404. Sodium (C10-13)-alkylbenzene sulfonate (47 %) (CAS No. 68411-30-3) applied on intact rabbit skin produced desquamation, necrosis and hyperkeratinisation by day 4 which persisted in all animals until day 10. The exposed areas had erythema and oedema which were not fully reversible within 14 days in 2 out of 3 animals.

Three studies were performed in accordance with the modified Draize test. LAS at concentrations of 1, 2.5 and 5 % was applied to intact rabbit skin under an occlusive dressing for 24 hours. Only the 5 % concentration caused adverse effects and it was considered a moderate irritant according to Draize criteria.

In a non-guideline study, MEA-C10-13 alkylbenzene sulfonate (undiluted) (CAS No. 85480-55-3) was severely irritating when applied to intact and abraded rabbit skin (application time unspecified). Severe primary irritation extending beyond the area of exposure was observed after the application of the test substance. At the final observation period, one week following treatment, skin sloughing with scar tissue formation was observed.

Eye Irritation

The eye irritation studies reported in OECD SIDS (2005), HERA (2013) and REACH (a,b) are consistent with the chemicals in this group causing serious eye damage at the tested concentrations of 47–50 %. Studies have also shown that LAS is moderately irritating at 5 % or more.

In four studies reported in OECD SIDS (2005), HERA (2013) and REACH(a), LASs (with CAS Nos 1322-98-1, 25155-30-0 and 68411-30-3) were reported to severely irritate the eyes of rabbits when tested according to OECD TG 405 at a concentration of 47–50 %. In one study, the exposure groups included: rinsed after 4 seconds, rinsed after 30 seconds and not rinsed. The effects were not reversible within 21 days in the unrinsed group but were fully reversible within 7 days for the 30 seconds rinsed group and 14 days for the 4 second rinsed group. In another study LAS (at 50 % concentration) was severely irritating to the eyes of rabbits. Adverse effects to the iris and conjunctivae were reported to persist to day 6.

LASs have also been tested at lower concentrations with varying severity of eye irritation observed. In two studies reported in HERA (2013) LASs were shown to be not irritating to the eye at concentrations of 0.01–1 %, but moderately irritating at 5 %.

However, in another two studies reported in HERA (2013) slight eye irritation was observed in animals treated with 0.01 % LAS, while considerable irritation of the conjunctivae was reported at 0.05 %. Adverse effects included severe irritation and oedema, turbidity of the cornea and disappearance of the corneal reflex. Effects were reversed completely after 120 h. However, irritation scores were not available.

MEA-C10-13 alkylbenzene sulfonate (CAS No. 85480-55-3) was reported to severely irritate the eyes of rabbits when tested similarly to OECD TG 405. Three groups of rabbits were used in the study; undiluted chemical without eye rinse, undiluted chemical with eye rinse after 4 seconds, and 10 % chemical without eye rinse. In the first group corneal opacity, vascularization of cornea and iritis were observed in all three animals. By day 14 pannus formation (two animals), and diffuse crimson red colouration of the conjunctivae and considerable eyelid swelling were observed in all three animals. Due to the severity of the reactions the animals were sacrificed. In the second group (rinsed), vascularisation of the cornea and iritis were observed in all animals and corneal opacity was not resolved by day 35 after treatment. In the third group (10 %) corneal opacities, iritis, and diffuse crimson red coloration of the conjunctivae with and without considerable swelling of the eyelids were observed in all three animals. All treated eyes in the third group recovered by day 14 (REACH b).

Observation in humans

Humans exposed to LAS have reported cases of skin irritation at dilute concentrations (IPCS 1996).

In two studies, primary skin irritation was induced by 1 % LAS (C12) in volunteers in a 24 hour closed patch test; erythema was observed. In another study the 1 % LAS (C12) was dripped onto the interdigital surface for 40 min once daily over two consecutive days; scaling was observed.

Sensitisation

Skin Sensitisation

In studies reported in HERA (2013), the negative results observed for the chemicals in several skin sensitisation animal studies (one guinea pig maximisation test (GPMT), one similar to GPMT, and one Buehler test) support a conclusion that the chemicals in this group are not skin sensitisers.

In the GPMT, LAS was applied at concentrations of 0.05 % (intracutaneous) and 1.5 % (topical). No positive reactions were reported for all test animals. In the study similar to GPMT, guinea pigs were tested with LAS at a concentration of 25 % intradermally and during the second topical induction one week later. The challenge exposure was performed at 12.5 % concentration. No positive reactions were reported for any test animal. In the Buehler study, animals were treated with LAS at an induction concentration of 1.0 % and challenge concentration of 0.8 %. No positive reactions were reported for any test animal.

Observation in humans

In human repeat insult patch tests (HRIPT) reported in HERA (2013), volunteers were treated with LAS at concentrations of 0.10 %w/v and 1 %w/v, in dilute preparations or product formulations. No evidence of skin sensitisation was found in subjects who completed the test.

In a HRIPT study reported in REACH (a,b), MEA-C10-13 alkylbenzene sulfonate (CAS No. 85480-55-3) was not found to induce skin sensitisation at a concentration of 0.05 %. However, repeated application of the chemical during the study produced irritation in 70/75 subjects.

Repeated Dose Toxicity

Oral

Based on the weight of evidence from the 15 repeated-dose toxicity studies with mice, rats and monkeys reported in OECD SIDS (2005) and IPCS (1996), the chemicals in this group do not cause serious damage to health by prolonged exposure if swallowed.

In oral gavage, dietary and drinking water studies in rats ranging between 28-days and 2-years, lowest observed adverse effect levels (LOAELs) of 115–750 mg/kg bw/day were reported. The no observed adverse effect levels (NOAELs) ranged from 40 to 250 mg/kg bw/day.

In the study reporting the lowest LOAEL, LAS was fed daily to Wistar rats for six months at concentrations from 0.07 to 1.8 %. Effects observed at higher concentrations included: 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 of the kidneys.

In the key study (where the highest NOAEL, 85 mg/kg bw/day, was reported below the lowest LOAEL), LAS was administered in drinking water daily to Wistar rats for nine months at concentrations from 0.07 to 0.6 %. Reduced body weight gain was observed in males in the high dose group. No organ weight changes were observed.

The monoethanolamine salts of LAS are not expected to show systemic toxicity based on the monoethanolamine functional group (NICNAS a).

Dermal

Based on the studies available for LAS by the dermal route, no adverse systemic effects are expected. However, the chemicals in this group may compromise the integrity of the skin and increase dermal absorption of other chemicals present in LAS-containing product formulations.

In a study reported in IPCS (1996), LAS (19.7 %) was applied to the dorsal skin of SLC-Wistar rats at doses ranging from 1–25 mg/rat, three times a week, for 24 months. The chemical was washed from the skin 24 hours after application. No treatment related changes in organ weights or histopathological parameters were recorded.

In a study reported in OECD SIDS (2005), LAS (20 and 30 %) was applied to the backs of male Wistar rats at doses of 286 and 427 mg/kg bw/day, daily, for 15 days. Body weight gain was reduced in the 20 % group and body weight decreased in the 30 % 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.

Inhalation

No data are available.

Genotoxicity

Based on the weight of evidence from the available in vitro and in vivo genotoxicity studies reported as well-conducted in OECD SIDS (2005) and IPCS (1996) on LASs (C10-14 and C10-13), the chemicals in this group are not considered to be genotoxic.

Negative results were reported in bacterial reverse mutation tests for mutagenicity to *Salmonella typhimurium* (strains TA1535, TA1537, TA1538, TA98 and TA100) and *Escherichia coli* (strain WP23uvrA) and a recombination assay against *Bacillus subtilis* (strains H17(rec+), M45(rec-)) with and without metabolic activation.

Negative results were reported in in vivo chromosomal aberration tests in ICR and ddY mice, and Wistar rats given oral doses up to 800 mg/kg bw/day or dietary doses up to 1170 mg/kg bw/day. In a mouse micronucleus assay, LAS did not induce a clastogenic effect.

The monoethanolamine salts of LAS are not expected to show genotoxicity based on the monoethanolamine functional group (NICNAS a).

Carcinogenicity

Based on the weight of evidence from the available carcinogenicity studies with rats reported in OECD SIDS (2005) and IPCS (1996), the chemicals in this group are not likely to be carcinogens. The IPCS monograph indicated that the studies were inadequate due to low group sizes, dose regimen, design factors and limited histological examination.

In four 2-year oral dietary or drinking water studies in rats, LAS (C10-14) was administered at maximum doses between 140 and 300 mg/kg bw/day. There was no gross or histopathological evidence of tumorigenesis nor any carcinogenic effect reported (OECD SIDS 2005).

Six studies were reported in IPCS (1996) in rats (Charles River and Wistar) which were fed LAS (C10-14) in the diet with maximum doses ranging between 250 and 1900 mg/kg bw/day for study durations between 6- and 24-months. In the two studies reported in the most detail, the high dose was 250 mg/kg bw/day; no treatment related histopathological effects or increased tumour incidences were observed. No evidence of tumorigenesis was reported in any of the studies.

The monoethanolamine salts of LAS are not expected to show carcinogenicity based on the monoethanolamine functional group (NICNAS a). An SCCS opinion notes that the salts of monethanolamines should not be used in cosmetic products containing *N*-nitrosating agents to prevent the formation of possibly carcinogenic nitrosamines (SCCS 2012).

Reproductive and Developmental Toxicity

Based on results of numerous reproductive and developmental toxicity studies in rats, mice and rabbits, a reported NOAEL of 85 mg/kg bw/day was determined for both maternal and developmental toxicity in rats. This was the highest NOAEL value below the lowest LOAEL value. The lowest maternal rat LOAEL of 115 mg/kg bw/day was associated with increased weight of the caecum and slight degeneration of the renal tubules (OECD SIDS 2005).

The IPCS monograph identified deficiencies in the studies including widely separated dose levels, limited dose levels (one or two), and studies on formulations. However, the OECD SIDS (2005) report considered the studies adequate for a weight of evidence approach.

There was no evidence of specific reproductive, fertility or developmental toxicity for LAS (C10-14) and a detergent containing 17 % LAS and 7 % alkyl ether sulfate, administered in dietary doses in 3- and 4-generation reproduction studies (OECD SIDS 2005). Based on the results, reported NOAELs of 70–350 mg/kg bw/day were determined for parental and offspring toxicity; these were the highest doses tested. General reproduction including fertility, gestation, neonatal viability, lactation, and post weaning growth was normal for all test groups and did not deviate from controls in two studies. In one study, statistically significant differences were occasionally observed in offspring but no dose related trends were observed over the three generations.

In 17 developmental toxicity studies where LAS was administered, adverse developmental effects were only observed at maternally toxic doses; these included embryo death or deformities and litter loss. 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) (OECD SIDS 2005).

The monoethanolamine salts of LAS are not expected to show specific reproductive or developmental toxicity based on the the monoethanolamine functional group (NICNAS a).

Risk Characterisation

Critical Health Effects

The critical health effects for risk characterisation include systemic acute effects (acute toxicity by the oral route of exposure) and local effects (eye damage and skin irritation). The chemicals in this group may also compromise the integrity of the skin and increase dermal absorption of other chemicals present in LAS containing product formulations.

Acute oral toxicity via damage to the mucous membranes has been reported in children exposed to high concentrations of chemicals in liquid laundry detergent capsules containing MEA dodecylbenzene sulfonate (CAS No. 26836-07-7).

Public Risk Characterisation

Sodium dodecylbenzene sulfonate (CAS No. 25155-30-0) is currently listed on Schedule 5 of the SUSMP for preparations containing 30 per cent or less of the chemical. At concentrations greater than 30 %, a number of warning statements, first aid instructions and safety directions apply.

Although use in cosmetic products in Australia has not been identified, international information indicates that some of the chemicals in this group are reported to be used in rinse-off cosmetic products at low concentrations (up to 5 %) (OECD SIDS 2005; CIR 2010). The concentration of the chemicals in laundry products in Australia has been identified at 10–30 % (SDS a-c) and up to 60 % in liquid laundry detergent capsules (SDS d).

Where high concentrations are used in domestic and potentially cosmetic products, the potential risk of accidental contact with the eye is a concern. Incidental oral exposure resulting in oral toxicity is considered less likely given the types of products in which the chemicals are used, with the exception of liquid laundry detergent capsules.

Accidental exposure of the chemicals to children, by ingestion and eye and skin contact, has occurred from liquid laundry detergent capsules, which rapidly dissolve in contact with moisture. In some cases referral to a hospital was required (Australian Competition and Consumer Commission (ACCC)). The likelihood of exposure in these cases is much greater than that expected from bulk packaged laundry detergents. The packaging format and fixed volume also enables rapid exposure to a concentrated dose of the chemicals. The ACCC has stated that the liquid laundry detergent capsules in their current form are highly attractive to children given the transparent packaging and bright colours. As there is some concern for children's safety, the ACCC and the relevant industry participants are working together to improve the safety and packaging of these products, should these chemicals be used in liquid laundry detergent capsules in their current form (Accord).

Additionally, the chemicals in this group are frequently formulated with related chemicals with similar toxicity including alcohol ethoxylates (NICNAS b), laureth sulfates (NICNAS c) and lauryl sulfates (NICNAS d). The cumulative toxicological effect on risk is also a concern. This should be taken into account when considering the appropriate regulatory framework for these chemicals.

Sodium dodecylbenzene sulfonate (CAS No. 25155-30-0) is currently risk managed through scheduling. While its toxicity profile suggest scheduling at lower concentrations (i.e. >5 %) under Schedule 5, this may not be necessary considering the longstanding and widespread pattern of use and community experience (NDPSC 1998), unless there is evidence to the contrary. However, there is a concern for the use of other chemicals in this group at higher concentrations and in liquid laundry detergent capsules without any regulatory controls.

The effects reported in the inhalation toxicity studies are not considered to be relevant to exposure to the public. The types of spray products (pump sprays) that contain the chemicals are designed to produce large particles to efficiently deliver the spray to the surface being cleaned. In practice, 95–99 % of cosmetic and commercial sprays have a mean aerodynamic equivalent diameter of >10 µm. This means the chemicals are more likely to have inhalable fractions that can be cleared through the mucociliary action of the lungs (CIR 2012).

Occupational Risk Characterisation

During product formulation, dermal, ocular and inhalation exposure of workers to the chemicals in this group may occur, particularly where manual or open processes are used. These may include transfer and blending activities, quality control analysis, and cleaning and maintenance of equipment. Worker exposure to the chemical at lower concentrations may also occur while using formulated products containing the chemical. The level and route of exposure will vary depending on the method of application and work practices employed.

Given the critical systemic acute and local health effects, the chemicals may pose an unreasonable risk to workers unless adequate control measures to minimise dermal, ocular and inhalation exposure to the chemicals are implemented. The

chemicals should be appropriately classified and labelled to ensure that a person conducting a business or undertaking (PCBU) at a workplace (such as an employer) has adequate information to determine appropriate controls.

The data available support an amendment to the hazard classification in HSIS (refer to **Recommendation section**).

NICNAS Recommendation

Further risk management is required. Sufficient information is available to recommend that risks to public health and safety from the potential use of the chemicals in cosmetics and/or domestic products be managed through changes to poisons scheduling, and risks for workplace health and safety be managed through changes to classification and labelling.

Assessment of the chemical is considered to be sufficient provided that risk management recommendations are implemented and all requirements are met under workplace health and safety and poisons legislation as adopted by the relevant state or territory.

Regulatory Control

Public Health

Appropriate scheduling and labelling should be undertaken to mitigate the risk from using the chemicals in this group in domestic and cosmetic products.

It is recommended that an amendment to the current listing of sodium dodecylbenzene sulfonate in Schedule 5 of the SUSMP be considered to include the other chemicals in this group given the same critical health effects and similar use pattern.

In addition, given the accidental ingestion and eye exposure in children to these chemicals when used in liquid laundry detergent capsules and the use of high concentrations of chemicals in this group in these formulations, consideration should also be given to whether additional scheduling measures are required for the chemicals in this group. Scheduling considerations should include:

- whether the chemicals in this group should be listed in Schedule 6 (where concentration exemptions may apply) when used in liquid laundry detergent capsules;
- the packaging and labelling requirements of the chemicals in domestic products; and
- the cumulative toxicological effect on risk of related chemicals with similar toxicity formulated in the same products.

However, these considerations should take into account voluntary actions already taken by industry to minimise accidental ingestion and eye exposure in children to liquid laundry detergent capsules.

Work Health and Safety

All the chemicals in the group are recommended for classification and labelling under the current approved criteria and adopted GHS as below. This assessment does not consider classification of physical hazards and environmental hazards.

Hazard	Approved Criteria (HSIS)[a]	GHS Classification (HCIS)[b]
Acute Toxicity	Harmful if swallowed (Xn; R22)*	Harmful if swallowed - Cat. 4 (H302)
Irritation / Corrosivity	Risk of serious eye damage (Xi; R41) Irritating to skin (Xi; R38)	Causes serious eye damage - Cat. 1 (H318) Causes skin irritation - Cat. 2 (H315)

[a] Approved Criteria for Classifying Hazardous Substances [NOHSC:1008(2004)].

[b] Globally Harmonized System of Classification and Labelling of Chemicals (GHS) United Nations, 2009. Third Edition.

[*] Existing Hazard Classification. No change recommended to this classification

Advice for consumers

Products containing chemicals in this group should be used according to the instructions on the label. In particular, parents and carers are advised to keep liquid laundry detergent capsules away from children and to follow the ACCC's specific advice in this regard on their website - Product Safety Australia.

Advice for industry

Control measures

Control measures to minimise the risk from oral, dermal, ocular and inhalation exposure to the chemical(s) should be implemented in accordance with the hierarchy of controls. Approaches to minimise risk include substitution, isolation and engineering controls. Measures required to eliminate or minimise risk arising from storing, handling and using a hazardous chemical depend on the physical form and the manner in which the chemical is used. Examples of control measures which may minimise the risk include, but are not limited to:

- using closed systems or isolating operations;
- using local exhaust ventilation to prevent the chemical from entering the breathing zone of any worker;
- minimising manual processes and work tasks through automating processes;
- work procedures that minimise splashes and spills;
- regularly cleaning equipment and work areas; and
- using protective equipment that is designed, constructed, and operated to ensure that the worker does not come into contact with the chemical.

Guidance on managing risks from hazardous chemicals are provided in the *Managing Risks of Hazardous Chemicals in the Workplace—Code of Practice* available on the Safe Work Australia website.

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. Guidance in selecting personal protective equipment can be obtained from Australian, Australian/New Zealand or other approved standards.

Obligations under workplace health and safety legislation

Information in this report should be taken into account to assist with meeting obligations under workplace health and safety legislation as adopted by the relevant state or territory. This includes, but is not limited to:

- ensuring that hazardous chemicals are correctly classified and labelled;
- ensuring that (material) safety data sheets ((m)SDS) containing accurate information about the hazards (relating to both health hazards and physicochemical (physical) hazards) of the chemical are prepared; and
- managing risks arising from storing, handling and using a hazardous chemical.

Your work health and safety regulator should be contacted for information on the work health and safety laws in your jurisdiction.

Information on how to prepare an (m)SDS and how to label containers of hazardous chemicals are provided in relevant codes of practice such as the *Preparation of Safety Data Sheets for Hazardous Chemicals— Code of Practice* and *Labelling of Workplace*

Hazardous Chemicals—Code of Practice, respectively. These codes of practice are available from the Safe Work Australia website.

A review of the physical hazards of the chemical has not been undertaken as part of this assessment.

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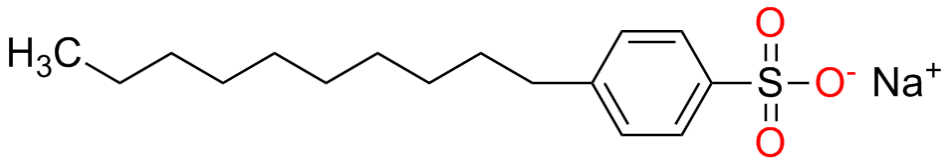
Last Update 07 February 2014

Chemical Identities

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, decyl-, sodium salt** sodium decylbenzene sulfonate
CAS Number	1322-98-1
Structural Formula	
Molecular Formula	C16H26O3S.Na
Molecular Weight	320.42

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, dodecyl-, ammonium salt** dodecylbenzenesulfonic acid, ammonium salt benzenesulfonic acid, dodecyl-, ammonium salt (1:1) ammonium dodecylbenzenesulfonate ammonium laurylbenzenesulfonate
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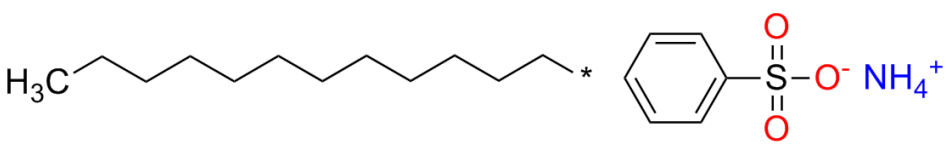
Structural Formula	
Molecular Formula	C18H30O3S.H3N

Molecular Weight	343.52

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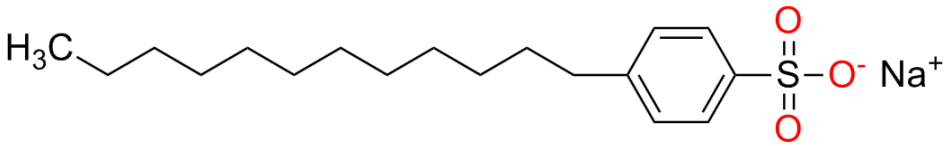
Structural Formula	
Molecular Formula	C18H30O3S.Na
Molecular Weight	349.48

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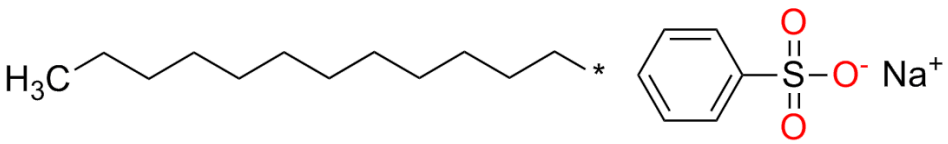
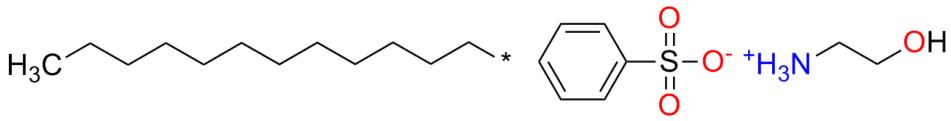
Structural Formula	
Molecular Formula	C18H30O3S.Na
Molecular Weight	349.48

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, dodecyl-, compound with 2-aminoethanol (1:1)** benzenesulfonic acid, dodecyl-, 2-aminoethanol salt (1:1) dodecylbenzenesulfonic acid, compound with 2-aminoethanol (1:1) dodecylbenzenesulfonic acid, monoethanolamine salt MEA dodecylbenzene sulfonate monoethanolamine dodecylbenzenesulfonate

CAS Number	26836-07-7
Structural Formula	
Molecular Formula	C18H30O3S.C2H7NO
Molecular Weight	387.58

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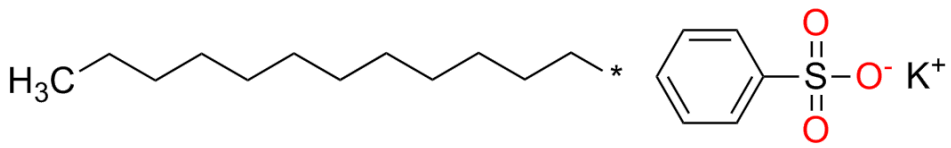
Structural Formula	
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Molecular Weight	365.59

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, 4-dodecyl-, compound with 2-aminoethanol (1:1)** monoethanolamine, p-dodecylbenzene sulfonate p-dodecylbenzenesulfonic acid, monoethanolamine salt 4-dodecylbenzenesulfonic acid, monoethanolamine salt MEA 4-dodecylbenzene sulfonate
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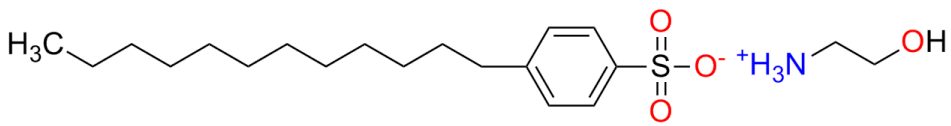
Structural Formula	
Molecular Formula	C18H30O3S.C2H7NO
Molecular Weight	387.58

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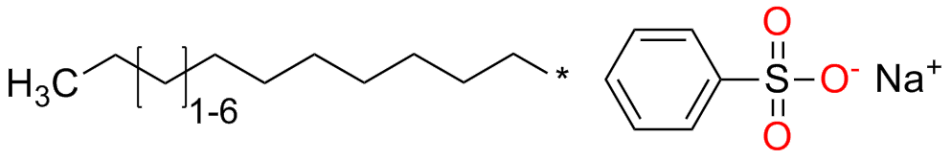
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

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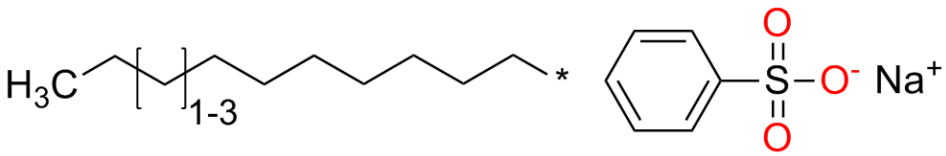
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

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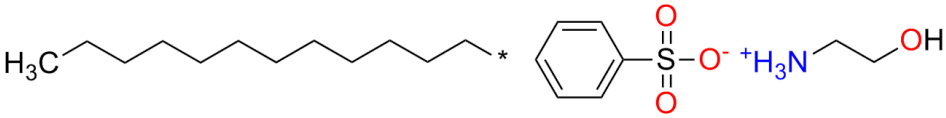
Structural Formula	

Molecular Formula	C18H30O3S.C2H7NO
Molecular Weight	387.58

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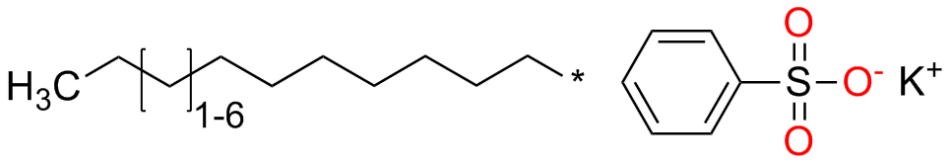
CAS Number	68584-27-0
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

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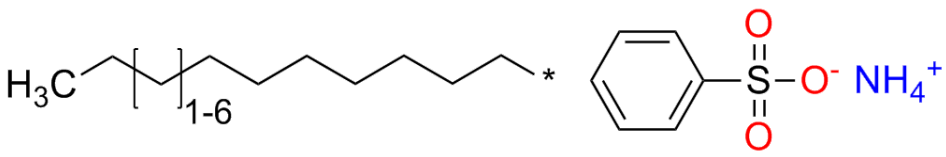
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, mono-C10-16-alkyl derivatives, compounds with 2-aminoethanol** (C10-16) alkylbenzenesulfonic acid, monoethanolamine salt MEA-C10-16 alkylbenzene sulfonate

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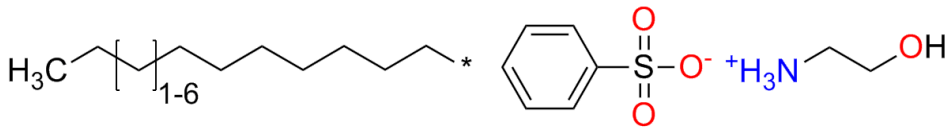
Structural Formula	
Molecular Formula	C6H6O3S.C2H7NO
Molecular Weight	Unspecified

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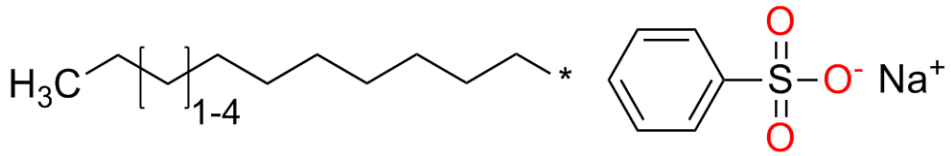
CAS Number	69669-44-9
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

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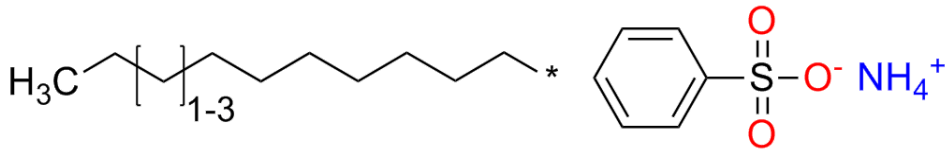
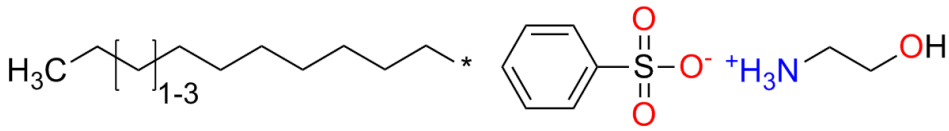
CAS Number	85480-54-2
Structural Formula	
Molecular Formula	Unspecified

Molecular Weight	

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, mono-C10-13-alkyl derivatives, compounds with ethanolamine** monoethanolamine mono-(C10-13)-alkylbenzene sulfonate MEA-C10-13 alkyl benzenesulfonate MEA dodecyl benzene sulfonate
CAS Number	85480-55-3
Structural Formula	
Molecular Formula	C6H6O3S.C2H7NO
Molecular Weight	Unspecified

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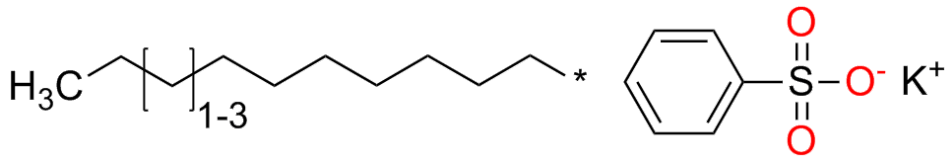
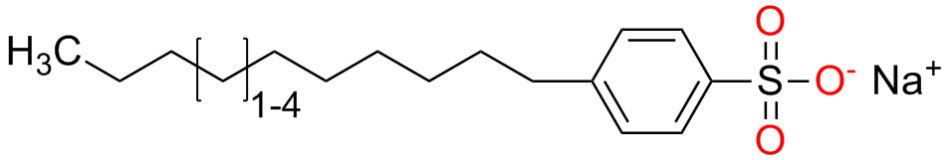
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

Chemical Name in the Inventory and Synonyms	**Benzenesulfonic acid, 4-C10-14-alkyl derivatives, sodium salts** sodium 4-(C10-14)-alkylbenzenesulfonate

CAS Number	91696-66-1
Structural Formula	
Molecular Formula	Unspecified
Molecular Weight	

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