


SIDS INITIAL ASSESSMENT PROFILE

CAS No.	27176-87-0
Chemical Name	Dodecylbenzenesulfonic acid
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR**Analogue Justification**

The Linear Alkylbenzene Sulfonate(LAS) category was assessed at SIAM 20. Data from the C12-LAS substances dodecylbenzene sulfonate and sodium dodecylbenzene sulfonate have been included in the assessment of Dodecylbenzenesulfonic acid for acute oral toxicity, skin and eye irritation, ready biodegradation, aquatic toxicity to fish and invertebrates endpoints.

Physical and chemical properties

Dodecylbenzenesulfonic acid (DBS) is a liquid organic substance (light yellow to brown). It has a melting point of 10°C and a boiling point of 460°C (calculated). An estimated pKa of 0.7 indicates that this acid is fully dissociated in the environmental pH range 4 to 9. Sodium dodecylbenzenesulfonate (CAS No. 25155-30-0) is a very close analogue of the dissociated acid because it readily dissociates in water and release the dodecylbenzene sulfonic anion in solution. Experimental aqueous solubility and log K_{OW} for this salt have been determined to be 300 mg/L and 1.96. A very low (modelled) vapour pressure of 3×10⁻¹³ Pa designates an acid with a negligible volatility.

Human Health

There is limited toxicokinetic information on DBS, which indicates uptake from the gastrointestinal tract was around 30% in a 5-week dietary administration study in rats. The main route of excretion was via the urine.

Low levels of Sodium dodecylbenzene sulfonate-derived residues were detected in all tissues analyzed on day 35 of the experiment. 8 male Wistar rats were given a single i.p. dose of 384.7 µg [¹⁴C]DBS in a 0.6% physiological NaCl solution. Within 10 days after dosing, rats excreted 94.5% of the dose applied, 84.7% in the first 24h.

The acute oral LD₅₀ in male/female rats is 650 mg/kg bw. No significant gross abnormalities were seen at autopsy. There is no available acute dermal and inhalation toxicity data for dodecylbenzenesulfonic acid.

Linear alkyl benzene sulfonate(LAS) was slightly irritating to the skin. Guinea-pig skin after 7 days exposure to LAS appeared shrunken, with thin layers of dermis and epidermis of guinea pigs in the histologic sections

compared to controls. A solution of 5% linear alkyl benzene sulfonate sodium salts, was slightly irritating to the eye of rabbit.

In a repeated dose oral toxicity study in rats [OECD TG 422], dodecylbenzenesulfonic acid was administered via gavage to male rats at 0, 100, 200, and 400 mg/kg bw/day, for from 2 weeks before mating to the end of the mating period (at least 28 days) and to female rats at 0, 100, 200, and 400 mg/kg bw/day, for from 2 weeks before mating to day 4 of lactation including the mating and gestation periods. One treatment-related death was observed in male rats in the high dose group. Oral administration of dodecylbenzenesulfonic acid to rats resulted in soft feces, and squamous cell hyperplasia of stomach in both sexes at 400mg/kg bw/day, and liquid feces and soiled perineal region, a decrease in body weight and food consumption in males at 400 mg/kg bw/day. In histopathological examination, squamous cell hyperplasia of stomach was observed in both sexes at 200 mg/kg bw/day and forestomach erosion/ulcer was observed in males at 400mg/kg bw/day. Based on these effects the NOAEL value was 100 mg/kg bw/day for male and female rats and the LOAEL value was 200 mg/kg bw/day for male and female rats. From these results, the target organ for oral dosing of dodecylbenzenesulfonic acid was considered to be the stomach.

In a bacterial reverse mutation assay [OECD TG 471], dodecylbenzenesulfonic acid was negative both with and without metabolic activation. An *in vitro* test chromosome aberration test [OECD TG 473] using Chinese hamster lung cells (CHL) was negative with and without metabolic activation. There was no data of *in vivo* test with dodecylbenzenesulfonic acid.

No data are available for the carcinogenicity of dodecylbenzenesulfonic acid.

In reproductive and developmental toxicity study performed according to the combined repeated dose toxicity study with the reproduction/developmental toxicity screening test [OECD TG 422], test conditions and dose were same as repeated dose toxicity. No treatment-related changes were observed in the copulation, fertility and pregnancy indices, gestation length, the number of corpora lutea and implantation, delivery index. Also no treatment - related changes were observed in all parameters of offsprings during the parturition and lactation periods. Based on these effects, the NOAEL for fertility and developmental toxicity was 400mg/kg bw/day, the highest dose tested.

Environment

For indirect photolysis in the atmosphere, the half-life of dodecylbenzenesulfonic acid is estimated to be 7.8hr (OH rate constant 16.36×10^{-12} cm³/ molecule-sec) with the AOPWIN model. Less than 10% hydrolysis was observed after 5 days at pH 4.0, 7.0 and 9.0 at 50±5 °C [OECD TG 111].

C12-LAS is readily biodegradable (more than 60% by mineralization within 28 days) [OECD TG 301 F].

Level III Fugacity modeling using EQC for a Type2 chemical, with equal releases to air, soil, and water shows the following percent distribution: air = 0.5%; soil = 65%; water = 32%; sediment = 2.5%. If released exclusively to water, the acid will primarily partition to water (93%) and sediment (7%). If released only to soil, it will remain in this compartment (100%). Results from calculations of environmental fate have to be considered with caution because the environmental partitioning of this substance is not exclusively function of its hydrophobicity, hence of its fugacity. For example, recent research shows that linear alkylbenzene sulfonates tend to partition to positively charged substrates in soils and sediments. A K_d value of 3210 L/kg has been determined for a C12 LAS in activated sludge with an organic carbon content of 26%. A K_{OC} value of 9076 has been obtained for a C12 LAS with the OECD TG 106 method. The estimated BCF of dodecylbenzenesulfonic acid is 70.79 with the BCFWIN model and experimental BCF values in fish, invertebrates and alga of sodium dodecylbenzenesulfonate ranged from 36 to 119. It suggests that dodecylbenzenesulfonic acid has a low potential for bioaccumulation.

Ecotoxicity data are available for dodecylbenzene sulfonic acid, C12 LAS and its salt with several comprehensive reviews having been completed.

The toxicity results from studies with aquatic organisms are as follows :

1) Acute toxicity :

Fish (*Salmo gairdnei*) / Dodecylbenzenesulfonic acid Na salts : 96 hr-LC₅₀ is 3.20-5.60 mg/L (nominal).

Invertebrates (*Daphnia magna*) / LAS : 48 hr-LC₅₀ is 3.5±1.0 mg/L(nominal).

Green algae (*Selenastrum capricornutum*) / Dodecylbenzenesulfonic acid: 72 hr-EC50(growth rate) is 65.4mg/L (measured) and 72 hr-EC50(yield) is 21.0 mg/L(measured). 72 hr-NOEC(growth rate and yield) is 7.9mg/L(measured)

Microorganism (activated sludge) / Na-12C LAS: 3hr-EC₅₀ is 500-723 mg/L(nominal).

2) Chronic toxicity :

Fish (*Pimephales promelas*) / C_{11.8} LAS : 1yr-NOEC is 0.90 mg/L(measured).

Invertebrates (*Daphnia magna*) /Sodium dodecylbenzene sulfonate : 21days-NOEC is 1.65 mg/L(nominal).

3) Soil dwelling organism

Lumbricus terrestris /LAS : 14days-LC₅₀ is 1.33mg/g(nominal).

Eisenia foetida / LAS : 14days-LC₅₀ > 1mg/g. (nominal).

Exposure

In the Republic of Korea estimated production amounts of dodecylbenzenesulfonic acid were approx. 89,460, 99,542, and 100,464 tons in 2005, 2006 and 2007, respectively. The estimated used amounts of the substance were approx. 7,410, 7,713, and 7,756 tons in 2005, 2006, and 2007, respectively. In Nordic countries estimated production amounts of this chemical were approx. 8,723, 12,522 and 10,400 tons in 2004, 2005 and 2006, respectively.

Dodecylbenzenesulfonic acid is used in production of detergents and in manufacturing of catalyser and as additives. Most of dodecylbenzenesulfonic acid that is used in industrial and consumer products as surfactant and ingredient in detergents will be disposed of by the sewerage system. Exposure to the environment may occur mainly via effluents of STP's and application of sewage sludge in agriculture.

In the Republic of Korea, dodecylbenzenesulfonic acid is produced by reacting SO₃ and LAB(linearalkylbenzene) in a continuous closed reactor. After this reaction is finished, atmosphere contaminants such as SO₂ and dust are emitted to atmosphere but the concentrations of the SO₂ and dust were below 10% level of environmental emission standard. All organic waste solvents occurred are burned by waste consignment treatment. Wastewater is treated chemically and biologically, and then it is discharged to wastewater treatment plant.

As for human exposure, in the sponsor country, this substance is produced in a continuous closed system and the manufacturing processes have been designed to maximize production yield and minimize potential releases. Good manufacturing design practices (e.g., enclosed production in agglomeration processes, exhaust ventilation and dust collection) and personal protective equipment in place at facilities that manufacture products are anticipated to mitigate worker exposure to this substance.

Dodecylbenzenesulfonic acid is the most common synthetic anion surfactant and it is usually used as an ingredient of detergents. Consumer can be exposure to dodecylbenzenesulfonic acid using detergents.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: The chemical is currently of low priority for further work because of its low hazard profile.

Environment: The chemical is currently of low priority for further work. The chemical possess properties indicating a hazard for the environment (acute aquatic toxicity to fish and invertebrates between 1 and 100 mg/L). However, the chemical does not warrant further work due to its ready biodegradation and limited potential for bioaccumulation.