FOREWORD INTRODUCTION

HYDROTROPES

CAS N°:

1300-72-7
12068-03-0
26447-10-9
28348-53-0
32073-22-6
37475-88-0

SIDS Initial Assessment Report

For

SIAM 21

18-20 October 2005, Washington DC, USA

1.	**Category Name:**	Hydrotropes
2.	**CAS Numbers:**	1300-72-7, 12068-03-0, 26447-10-9, 28348-53-0, 32073-22-6, 37475-88-0
3.	**Sponsor Country:**	Australia Contact person: Dr Sneha Satya Team Leader Review & Treaties NICNAS 334-336 Illawarra Road Marrickville, NSW 2204 Australia Ph: +61 2 8577 8880 Fax: +61 2 8577 8888
4.	**Shared Partnership with:**	Hydrotropes Consortium Contact person: Kathleen Stanton Consortium Manager The Soap and Detergent Association 1500 K Street, N.W., Suite 300 Washington, D.C. 20005 USA Tel: (202) 662-2513 Fax: (202) 347-4110
5.	**Roles/Responsibilities of the Partners:**	Industry Consortia prepared the initial documents. The National Industrial Chemicals Notification and Assessment Scheme (NICNAS), Australian Government Department of Health and Ageing was the main reviewer. The environmental sections were reviewed by the Australian Government Department of the Environment and Heritage (ADEH).
•	Name of industry sponsor	Hydrotropes Consortium

/consortium

- Process used

Consortium member companies contributed in-house studies of physical-chemical properties, environmental fate and transport, ecotoxicity and mammalian toxicity for the chemicals in the category. To supplement the industry data, literature searches were conducted of on-line databases available from the U.S. Chemical Information Systems, the European International Uniform Chemical Information Database [IUCLID], the Institute for Systems, Informatics and Safety, and Environmental Chemicals Data Information Network (e.g., Hazardous Substances Databank [HSDB], Registry of Toxic Effects of Chemical Substances [RTECS], Toxic Substances Control Act Test Submissions [TSCATS], Integrated Risk Information System [IRIS], Chemical Carcinogenesis Research Information [CCRIS], GENETOX, The Environmental Mutagen Information Center [EMIC], The Environmental Teratology Information Center [ETIC], The Developmental and Reproduction Toxicology Database [DART], The Catalog of Teratogenic Agents [CTA], ENVIROFATE, DATALOG, PHYTOTOX, TERRATOX and Aquatic Toxicity Information Retrieval [AQUIRE]), and standard scientific data compendia (e.g., CRC Handbook of Chemistry and Physics, and The Merck Index). The sum total of the in-house studies, reference books, and literature searches of on-line databases was the identification of a substantial amount of available data.

All data/reports identified were subject to a reliability evaluation using the Klimisch Criteria to assign data adequacy for the HPV/SIDS profile. NICNAS conducted an independent literature search to ensure all available studies were included. The Consortium prepared first drafts and NICNAS and ADEH reviewed and edited drafts to achieve the final document.

6. Sponsorship History

- How was the chemical or category brought into the OECD HPV Chemicals Programme ?

The industry coalition agreed to sponsor hydrotropes in the SIDS-International Council of Chemical Associations (ICCA) Program, with Australia being the sponsor country.

7. Review Process Prior to the SIAM:

Prepared by industry. Reviewed and edited by NICNAS and ADEH to reach a consensus document.

8. Quality check process:

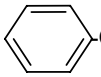
Industry coalition members developed the draft documents, which were then reviewed by the sponsor country.

9. Date of Submission:

22 July 2005

10. Comments:

SIDS INITIAL ASSESSMENT PROFILE

CAS Nos. **and** **Chemical names**	(**1300-72-7** and 827-21-4) Xylenesulfonic acid, sodium salt (**12068-03-0**) Toluenesulfonic acid, sodium salt (**26447-10-9**) Xylenesulfonic acid, ammonium salt (**28348-53-0** and **32073-22-6**) Cumenesulfonic acid, sodium salt (**37475-88-0**) Cumenesulfonic acid, ammonium salt (28088-63-3) Xylenesulfonic acid, calcium salt (30346-73-7) Xylenesulfonic acid, potassium salt (16106-44-8) Toluenesulfonic acid, potassium salt **The 6 compounds in** bold **are sponsored HPV chemicals; the remaining 4 compounds are supporting/supported chemicals in the category.**
Category Name	**Hydrotropes**
Structural Formulas	 $-CH_3$ $-SO_3Na$ toluene sulfonic acid, sodium salt  $-(CH_3)_2$ $-SO_3Na$ xylene sulfonic acid, sodium salt  $-CH.(CH_3)_2$ $-SO_3Na$ cumene sulfonic acid, sodium salt The category also includes isomeric forms (ortho, meta, and/or para) of the respective sulfonic acid salts (sodium, ammonium, calcium and potassium).

SUMMARY CONCLUSIONS OF THE SIAR

Category Identification/ Justification

Hydrotropes are supported as a category because of the close consistency of the compounds, their commercial uses, fate, and health and environmental effects. The hydrotropes are used as coupling agents to solubilize the water insoluble and often incompatible functional ingredients of household and institutional cleaning products and personal care products. These hydrotropes are not surfactants but are used to solubilize complex formulas in water. They function to stabilize solutions, modify viscosity and cloud-point, limit low temperature phase separation and reduce foam formation. Manufactured products are used as aqueous solutions (30-60% active

substance) or as granular solids containing 90-95% active substance.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+). Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has led to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicological properties of these chemical entities are essentially the same.

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

It was therefore concluded that the three sub-groups are expected to be generally comparable and predictable in their chemical behavior (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

Human Health

Toxicological studies have been conducted with numerous members of the hydrotropes category. Data on all SIDS-endpoints are available and indicate a relatively low toxicity for these compounds.

No studies on absorption, distribution, metabolism and elimination for the hydrotropes category were identified. However, based on the physico-chemical properties such as molecular weight, water solubility and octanol-water partition coefficient, and the available toxicological studies, it can be concluded that significant absorption occurs following oral administration while absorption following dermal application is limited.

Across the hydrotropes category, toxicity results are consistent across the toluene, xylene and cumene sulfonates and their various salts. The acute oral LD50 in rats ranges from 1044 mg a.i./kg bw (calcium xylene sulfonate) to 6500 mg a.i./kg bw (sodium xylene sulfonate), , the dermal LD50 in rabbits is >624 mg a.i./kg bw (calcium xylene sulfonate), and the inhalation LC50 in rats is >557 mg/L (557 g/m^3 sodium toluene sulfonate) and in rabbits >6.41 mg/L (6.41 g/m^3 ammonium xylene sulfonate). The inhalation studies are from secondary sources. Clinical signs observed in acute oral toxicity studies included decreased activity, weakness, prostration, increased salivation, diarrhea, ptosis and anogenital staining. Necropsy findings reported in these same studies included slight pulmonary inflammation, gastrointestinal inflammation and hemorrhage, mild liver changes, congestion of liver, kidneys, adrenal glands an gastrointestinal tract, and redness of stomach mucosa in animals that died. Observations were within normal limits with a report of slight to moderate congestion of adrenal glands in animals that survived. Clinical signs observed in acute dermal exposure included erythema with additional desquamation. At necropsy findings reported were focal or multifocal red discoloration and desquamation of the treated skin.

A series of rabbit skin and eye irritation studies are reported for members of the hydrotropes category. Sodium xylene sulfonate is not a skin irritant. Calcium xylene sulfonate and sodium cumene sulfonate are not skin irritants and both caused slight but reversible eye irritation. There is no indication of skin sensitization for the hydrotropes category based on the available animal (GLP Buehler study). No reliable human data are available for sensitization.

Thirteen oral and dermal repeat dose toxicity studies (subchronic and chronic) conducted in rats or mice are available for the hydrotropes category. Test durations ranged from 17 days up to 2 years and exposure doses ranged from 6 to 2000 mg a.i. /kg bw/day sodium xylene sulphonate by the dermal route and from 1.1 up to 4092 mg a.i./kg bw/day sodium xylene sulphonate by the oral route. No significant systemic toxicity was observed in any of the dermal studies. Local effects were reported in one of six dermal studies. In that study the LOAEL was 1300 mg a.i./kg bw/day of sodium xylene sulphonate and the adverse effect was epidermal hyperplasia at the site

of application in both male and female mice.. The corresponding NOAEL was 440 mg a.i./kg bw/day.. In the same study, the mean body weight gain of the high dose males was significantly greater (105%) than that of the control group. This change was not considered to be biologically significant by the authors (US National Institute of Health).

One of the eight oral repeat dose studies reported a 17% (statistically significant) decrease in relative spleen weight in female rats exposed 90 days to sodium xylene sulfonate. No adverse effects were reported in males. The LOAEL for this study was 4092 mg a.i./kg bw/day and the NOAEL was 763 mg a.i./kg bw/day. A 12% (statistically significant) reduction in body weight gain of female rats was reported in an older (1968) 91-day oral study with sodium cumene sulfonate at the dose level of 159 mg a.i./kg bw/day. No effects were observed in male rats. The study report stated that the decrease in body weight gain for females was within the established ranges for animals of this species and age and was therefore not considered an adverse effect by the authors. The decrease in body weight gain wasnot associated with any other effects. Two more recent (1980) and well reported 90 day studies with rats and mice exposed to sodium xylene sulfonate did not report a reduction in body weight gain at much higher doses, and consequently the effect in the sodium cumene sulfonate study is considered questionable. The most appropriate NOAEL for systemic toxicity from mammalian toxicity studies was therefore determined to be 763 mg a.i./kg bw/day based on a reduction in relative spleen weight in female rats.

The hydrotropes category has been assessed for mutagenic potential in a variety of *in vivo* and *in vitro* assays. Specifically mouse micronucleus cytogenetic assays with calcium xylene sulfonate and sodium cumene sulfonate, Ames assay with calcium xylene sulphonate, sodium cumene sulphonate and sodium xylene sulphonate and mouse lymphoma, sister chromatid exchange, and chromosome aberration assays with sodium xylene sulfonate. No positive results were seen *in vitro* or *in vivo* in any of the studies. Thus the available data indicate that the chemicals in the hydrotropes category do not have a genotoxic potential.

Chronic toxicity/carcinogenicity data exist for the hydrotropes category for both rats and mice dermally exposed for 2 years. There was no evidence of a carcinogenic potential for the hydrotropes category in these dermal exposure studies. It is noted that there is limited dermal absorption of hydrotropes.

No reproductive toxicity studies are reported for the hydrotropes category. However, the 91-day oral rat feeding study with sodium cumene sulfonate, the 90-day feeding study with sodium xylene sulfonate and the 90-day and 2-year dermal studies with sodium xylene sulfonate included examination of sex organs such as the prostate, testes and ovaries. There is no evidence from these repeat dose studies to suggest that these chemicals would have an adverse effect on reproductive organs.

Calcium xylene sulfonate has been evaluated for the potential to cause developmental toxicity in rats. Calcium xylene sulfonate (31% a.i.) was administered via gavage to female rats (30 per dose) at 0, 150, 1500 or 3000 mg/kg bw in water on days 6 to 15 of gestation. This study followed the US EPA TSCA Guideline 1985. Only one animal died during the study (mid-dose). No treatment related effects were observed. An increase in food intake observed at the highest dose was considered to be within ranges of biological variation for this species. There was no evidence of developmental toxicity in rats. The NOAEL for maternal and foetal toxicity was the highest dose tested at 3000 mg/kg bw/day (corresponding to 936 mg a.i./kg bw/day).

Environment

Hydrotropes are solid at ambient temperatures. Melting point experiments were carried out with calcium xylene sulfonate and sodium toluene sulfonate. Calcium xylene sulfonate decomposed in a melting point experiment at a temperature between 100°C and 375°C. No clear melting point was observed up to 300°C with sodium toluene sulfonate. Modelled estimates across the range of hydrotropes for melting points are in excess of 200°C and boiling points are in excess of 450°C. Hydrotropes are water soluble (>1000 mg/L) and have low volatility with a vapour pressure of $<2.0 \times 10^{-5}$ Pa for sodium xylene sulfonate at 25°C (vapour pressure was measured at 240-250^{o}C and extrapolated to 25°C). A measured octanol-water partition coefficient (logKow) value of -2.7 exists for calcium xylene sulfonate, which correlates with modeled logKow estimations ranging between -2.4 and -1.5 for the sodium xylene, toluene and cumene sulfonates. Fugacity modelling across the range of hydrotropes predicts a 99+% residence in the water compartment following environmental release.
Biodegradation constitutes the primary elimination mechanism from the environment. Studies across the hydrotropes category demonstrate rapid and complete biodegradation under aerobic conditions and the hydrotropes are considered to be readily biodegradable according to OECD criteria. No data are available on anaerobic degradation. There is photodegradation potential for hydrotropes based upon modelled atmospheric oxidation half-lives of 40 hours for the cumene sulfonates, 41 hours for the xylene sulfonates, and 105 hours for

the toluene sulfonates. Hydrotropes are not subject to hydrolysis. Commercial products containing hydrotropes are often aqueous solutions and they are stable. Removal of hydrotropes from secondary activated sludge sewage treatment processes is greater than 94%, as observed in a modified SCAS study with calcium xylene sulfonate. Bacterial toxicity studies indicate that the hydrotropes category is not expected to negatively impact sewage treatment microorganisms. Fish bioconcentration studies conducted at two exposure concentrations with sodium xylene sulfonate and sodium toluene sulfonate reported BCF values of <2.3. Model predictions using the measured and estimated log Kow values of -2.7 to -1.5 also indicate low bioaccumulation potential. The highest estimated Bioconcentration Factor [BCF] was approximately 3. Monitoring data are not available for the hydrotropes category.

Reliable ecotoxicity data are available on all SIDS-endpoints for selected members of the category. The data cover fish, invertebrates and algae for xylene sulfonate (sodium, ammonium and calcium salts) and cumene sulfonate (sodium salt). While the toluene benzene derivative is not represented in the available data set, results are consistent for the chemicals tested, providing confidence in the ability to read-across for other category members. Based on hazard data, aquatic toxicity is considered to be uniformly low across the hydrotropes category.

Fish acute LC_{50} values are >400 mg/L in six studies. *Daphnia* acute EC_{50} values are >318 mg/L in five studies. The acute LC_{50} to the marine invertebrate *Artemia* is >400 mg/L in one study. Freshwater green algae are considered the most sensitive species with EC_{50} values ranging between 230-236 mg a.i./L and No Observed Effect Concentrations (NOECs) ranging between 31-75 mg a.i./L. The 48-hr EC10 for the bacteria *Pseudomonas putida* exposed in a Bringmann-Kuehn-Test is reported as >16,000 mg/L sodium cumene sulfonate. A daphnid 21-day chronic toxicity NOEC value of approximately 30 mg/L has been reported for sodium cumene sulfonate, however the data is sourced from secondary literature with limited reliability.

The suggested aquatic Predicted No Effect Concentration (PNEC) is 2.3 mg/L calculated as the lowest EC_{50} for three species (algae, fish, daphnia) divided by an assessment factor of 100. The lowest EC_{50} is 230 mg/L (based on algal toxicity for sodium xylene sulfonate), this divided by 100 equals 2.3 mg/L. A PNEC of 2.3mg/L is consistent with what would be predicted using the chronic daphnia NOEC divided by 10, or using the 96-hour algal NOEC as a chronic endpoint divided by 10.

Exposure

Current hydrotrope volumes (production + importation) based on 100% active material are approximately 29,000 metric tonnes in the U.S., 1,100 metric tonnes (40% concentration) in Australia, and 19,000 metric tonnes in Europe. Hydrotropes are used at active concentrations between 0.1 and 15% in consumer cleaning and personal care products. They function as coupling agents in liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. In Australia, a relatively small volume (about 55 tonnes per year) is used in liquid sulphur textile dyes present at 7.5 – 50%, acidic recirculation cleaning products present at 10-25%, wetting agent for tanning industry present at 10%, enzymatic recirculation cleaner for dairy and food processing applications at 4%, coolant system conditioner at 6.9%, car wash detergents at 1.3–6.3%, cleaners and degreasers at 0.1–6.3%, vinyl, plastic rubber restorer at 0.2% and floor stripper at 2.7–9 %. There are no industrial process intermediate uses of the hydrotropes.

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for the hydrotropes category. No workplace air monitoring data are available.

Hydrotropes are used in consumer/professional cleaning and personal care products, which may be used “as is”, or diluted prior to or during use. Dermal contact will occur with these products. There is some potential for incidental or accidental ingestion of, inhalation of, and/or eye contact with products during handling and use. Exposure to hydrotropes in formulated consumer products is mitigated by following use and precaution

instructions on product labels. Human exposure will be mitigated by the fact that residues from many of these products are washed or rinsed off.

Environmental releases from production facilities and from down-the-drain discharges following product use may lead to potential environmental exposures in surface waters and indirect human exposures via drinking water and/or fish consumption. Environmental exposure will be mitigated by the fact that hydrotropes, which reside predominantly in the water compartment, are readily biodegraded and are removed to a large degree during wastewater treatment and have low potential for bioaccumulation.

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

Human Health: The chemicals in this category are of low priority for further work because of their low hazard profile.

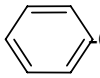
Environment: The chemicals in this category are of low priority for further work because of their low hazard profile.

SIDS Initial Assessment Report

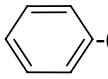
1 IDENTITY

Compounds known as hydrotropes are amphiphilic substances composed of both a hydrophilic and a hydrophobic functional group. The hydrophobic part of the molecule is a benzene substituted (i.e., methyl [common name: toluene], dimethyl [common name: xylene] or methylethyl [common name: cumene] apolar segment. The hydrophilic, polar segment is an anionic sulfonate group accompanied by a counter ion (e.g., sodium and ammonium). This segment is a comparatively short side-chain as seen in the diagrams below. There are 6 sponsored hydrotropes.

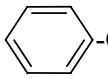
Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate or hydrotrope. Commercial toluene (and cumene) sulfonates consist of mixtures of 3 isomers (ortho-, meta- and para-). Commercial xylene sulfonic acid consists of mixtures of 6 isomers (ortho,ortho, meta,meta, para,para, ortho,meta, ortho,para, and meta,para). Diagrams of sodium salts for each of the three hydrotropes (without isomer orientation) are depicted below. An ortho-isomer would have adjacent attachment points to the benzene ring; a para-isomer would have attachments at opposite ends of the benzene ring; and a meta-isomer would have one open carbon between attachments on the benzene ring.



toluene sulfonic acid, sodium salt



xylene sulfonic acid, sodium salt



cumene sulfonic acid, sodium salt

The hydrotropes are used as coupling agents to solubilize the water insoluble and often incompatible functional ingredients of household and institutional cleaning products and personal care products. These hydrotropes are not surfactants but are used to solubilize complex formulas in water. They function to stabilize solutions, modify viscosity and cloud-point, limit low temperature phase separation and reduce foam formation. Manufactured products are used as aqueous solutions (30-60% active substance) or as granular solids containing 90-95% active substance.

1.1 Identification of the Substance Category

Chemical Abstracts Service (CAS) Numbers:	1300-72-7, 12068-03-0, 26447-10-9, 28348-53-0, 32073-22-6 and 37475-88-0. In addition to the six sponsored chemicals listed above, the following four additional substances provide supporting data and are supported by the data in this SIAR: 827-21-4, 28088-63-3, 30346-73-7, 16106-44-8.
International Union of Pure and Applied Chemistry (IUPAC) Name:	(1300-72-7 and 827-21-4) Xylenesulfonic acid, sodium salt; (12068-03-0) Toluenesulfonic acid, sodium salt; (26447-10-9) Xylenesulfonic acid, ammonium salt; (28348-53-0 and 32073-22-6) Cumenesulfonic acid, sodium salt; (37475-88-0) Cumenesulfonic acid, ammonium salt; (28088-63-3) Xylenesulfonic acid, calcium salt; (30346-73-7) Xylenesulfonic

acid, potassium salt; and (16106-44-8) Toluenesulfonic acid, potassium salt.

Description: The category is represented by six sponsored (and four additional supporting) hydrotropes that are amphiphilic substances composed of a hydrophobic, benzene substituted, apolar segment and a hydrophilic, anionic sulfonate, polar segment. The commercial substances can be sodium, ammonium, potassium or calcium salts. The category describes these hydrotropes that are amphiphilic coupling agents used in a wide range of cleaning and personal care products.

Molecular Formula: $C_7H_8O_3S$[Na or NH_4 or Ca or K] *to* $C_9H_{12}O_3S$[Na or NH_4or Ca or K]

Structural Formula: C_6H_3 . CH_3 . SO_3[Na or etc.] *to* C_6H_3 . $(CH_3)_3$. SO_3[Na or etc.]

Molecular Weight: 194 to 226

Synonyms: 1300-72-7 and 827-21-4: Xylenesulfonic acid, sodium salt; xylenesulfonate, sodium salt; sodium xylene sulfonate; Benzenesulfonic acid (1-dimentyl) sodium salt; dimethylbenzenesulfonate, sodium salt

12068-03-0: Toluenesulfonic acid, sodium salt; toluene sulfonate, sodium salt; sodium toluene sulfonate; benzenesulfonic acid (1-methyl) sodium salt; methylbenzenesulfonate, sodium salt

26447-10-9: Xylenesulfonic acid, ammonium salt; xylenesulfonate, ammonium salt; ammonium xylene sulfonate; Benzenesulfonic acid (1-dimentyl) ammonium salt; dimethylbenzenesulfonate, ammonium salt

28348-53-0 and 32073-22-6: Cumenesulfonic acid, sodium salt; cumenesulfonate, sodium salt; sodium cumene sulfonate; Benzenesulfonic acid (1 methylethyl) sodium salt; methylethylbenzenesulfonate, sodium salt

37475-88-0: Cumenesulfonic acid, ammonium salt; cumenesulfonate, ammonium salt; ammonium cumene sulfonate; Benzenesulfonic acid (1 methylethyl) ammonium salt; methylethylbenzenesulfonate, ammonium salt

28088-63-3: Xylenesulfonic acid, calcium salt; xylenesulfonate, calcium salt; calcium xylene sulfonate; Benzenesulfonic acid (1-dimentyl) calcium salt; dimethylbenzenesulfonate, calcium salt

30346-73-7: Xylenesulfonic acid, potassium salt; xylenesulfonate, potassium salt; potassium xylene sulfonate; Benzenesulfonic acid (1-dimentyl) potassium salt; dimethylbenzenesulfonate, potassium salt

16106-44-8: Toluenesulfonic acid, potassium salt; toluene sulfonate, potassium salt; potassium toluene sulfonate; benzenesulfonic acid (1-methyl) potassium salt; methylbenzenesulfonate, potassium salt

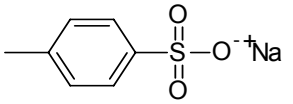
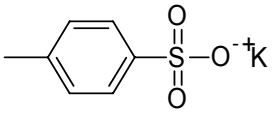
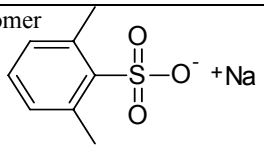
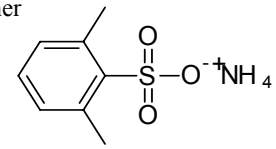
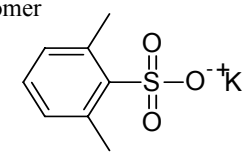
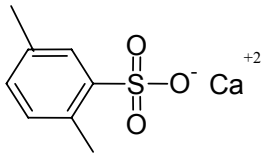
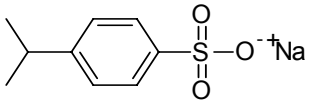
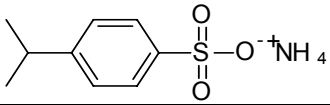
Category Justification for Hydrotropes:

The six sponsored hydrotropes have High Production Volume (HPV) chemical status in one or more OECD regions. However, the Hydrotropes Consortium has identified a total of four additional hydrotrope substances that are analogues to the six sponsored materials and are also supported by the HPV data. In two cases (CAS Nos. 28088-63-3 and 16106-44-8) these substances provide supporting data for the chemical category. Therefore all ten chemicals (six as sponsored

chemicals and four as supporting chemicals) are included in this SIAR for the purpose of defining and evaluating the chemical category.

The chemicals within the category "hydrotropes" including chemical name, CAS No. and a representative structure of the commercial mixture (isomer identified) are shown in Table 1.

Table 1: Category of Hydrotropes

Chemical Name	CAS No.	Structure
Toluene sulfonic acid, sodium salt	**12068-03-0**	para isomer 
Toluene sulfonic acid, potassium salt	16106-44-8	para isomer 
Xylene sulfonic acid, sodium salt	**1300-72-7** 827-21-4	ortho,ortho isomer 
Xylene sulfonic acid, ammonium salt	**26447-10-9**	ortho,ortho isomer 
Xylene sulfonic acid, potassium salt	30346-73-7	ortho,ortho isomer 
Xylene sulfonic acid, calcium salt	28088-63-3	meta,ortho isomer 
Cumene sulfonic acid, sodium salt	**28348-53-0** **32073-22-6**	para isomer 
Cumene sulfonic acid, ammonium salt	**37475-88-0**	para isomer 

*** Sponsored HPV chemicals are shown in bold**. Other substances are supporting compounds.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in

counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+). Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in aqueous solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

It was therefore concluded that the three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

Some of these molecules also exist under the acid form and are commercial products. These products are not ICCA Initiative HPVC, but their chemical structures are close enough that extrapolating some of the test results may be appropriate from the neutralized forms. This is particularly true for tests done under high dilution in water with a pH control (for example, most of the ecotoxicology tests).

1.2 Purity/Impurities/Additives

The hydrotropes are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

1.3 Physico-Chemical properties

Table 2 provides the available measured physico-chemical properties for members of the hydrotropes category as well as modelled values using the EPIWIN model available at http://www.epa.gov/opptintr/exposure/docs/episuite.htm for those properties lacking measured values. Measured values are typically preferred over modelled values, however, modelled values can provide reasonably accurate directions/trends (e.g., relatively high or low) for these properties.

Measurements show hydrotropes to be relatively highly soluble in water. Hydrotropes are ionic solids and boiling and melting points are expected to be high. Measurements were done with samples that were between 88 and greater than 93% pure, resulting in melting points ranging from 182°C to >375°C. Modelled data show that the category has very narrow ranges for both melting and boiling points, between 198-247°C and 468-549°C, respectively. Vapour pressure was measured at less than (<) 2.0×10^{-5} Pa in a recent guideline study. Modelled estimates of vapour pressure are lower; ranging from 1.1×10^{-9} to 3.56×10^{-7} Pa. These relatively low measured and modelled values indicate very slight volatility (Mensink et al., 1995) and are consistent with a 2000 IUCLID data sheet indicating hydrotropes to be “non-volatile”. The lower measured value is a limit value only, thus its variance from modelled data is not unexpected. The single measured

octanol:water partition coefficient is low and consistent with modelled estimates. Modelled estimates are between 0.23 and -2.4, indicating that the properties of the individual chemicals are consistent over the category. The narrow ranges for all data, both measured and modeled for the category, indicates that the chemicals have very similar physical and chemical properties.

Table 2: Measured and Modelled Physico-Chemical Properties of Hydrotropes Category

Property	Compound	CAS No.	Modelled Value	Measured Value	Reference[1]
Physical state	Pure	All	-	Solid at room temperature	Albright & Wilson Americas Inc., 1997; Rutgers Organics Corporation, 1997a, b, c, d
Melting point	Xylene sulfonate, Na	1300-72-7	233° C	>300° C	EPI (2); Rutgers Organics Corporation, 1997a (4)
	Xylene sulfonate, Na	827-21-4	233° C	>300° C	EPI (2); CERI, 1996a (2)
	Xylene sulfonate, Ca	28088-63-3	247° C	>375 ° C	Ruetgers-Nease Chemical, Inc., 1997a (1)
	Cumene sulfonate, Na	28348-53-0	236° C	182° C and >300° C	EPI (2); Albright & Wilson Americas Inc., 1997 (4); Rutgers Organics Corporation, 1997c (4)
	Toluene sulfonate, Na	12068-03-0	228° C	>300° C	EPI (2), CERI, 1996b (2)
	Xylene sulfonate, NH_4	26447-10-9	198° C	-	EPI (2)
	Cumene sulfonate, NH_4	37475-88-0	200° C	-	EPI (2)
	Xylene sulfonate, K	30346-73-7	233° C	-	EPI (2)
	Toluene sulfonate, K	16106-44-8	228° C	-	EPI (2)
Boiling point	Xylene sulfonate, Na	1300-72-7	545° C	-	EPI (2)
	Xylene sulfonate, NH_4	26447-10-9	468° C	-	EPI (2)
	Toluene sulfonate, Na	12068-03-0	533° C	-	EPI (2)
	Cumene sulfonate, NH_4	37475-88-0	473° C	-	EPI (2)
	Cumene sulfonate, Na	28348-53-0	549° C	-	EPI (2)
	Xylene sulfonate, Ca	28088-63-3	545° C	-	EPI (2)
	Xylene sulfonate, K	30346-73-7	545° C	-	EPI (2)
	Toluene sulfonate, K	16106-44-8	533° C	-	EPI (2)
Relative density	Xylene sulfonate, Na	1300-72-7		1.02-1.08	Albright & Wilson, Ltd., 2000 (4)
	Xylene sulfonate, Ca	28088-63-3		1.3	Ruetgers-Nease Chemical., 1996 (1)
Vapour pressure	Xylene sulfonate, Na	1300-72-7	2.03 $x10^{-7}$ Pa	Non-volatile <2.0 $x10^{-5}$ Pa	EPI (2), Albright & Wilson, Ltd., 2000 (4), SafePharm Labs, 2005 (1)
	Xylene sulfonate, Ca	28088-63-3	1.6 $x10^{-9}$ Pa	-	EPI (2)
	Toluene sulfonate, Na	12068-03-0	3.47 $x10^{-9}$ Pa	-	EPI (2)
	Cumene sulfonate, Na	28348-53-0	1.09 $x10^{-9}$ Pa	-	EPI (2)
	Xylene sulfonate, NH_4	26447-10-9	3.56 $x10^{-7}$ Pa	-	EPI (2)
	Cumene sulfonate, NH_4	37475-88-0	2.57 $x10^{-7}$ Pa	-	EPI (2)
	Xylene sulfonate, K	30346-73-7	2.03 $x10^{-7}$ Pa	-	EPI (2)
	Toluene sulfonate, K	16106-44-8	3.51 $x10^{-9}$ Pa	-	EPI (2)
Water solubility	Toluene sulfonate, Na	12068-03-0	1000 g/L	Soluble	EPI (2); Rutgers Organics Corporation, 1997d (4)
	Xylene sulfonate, Na	1300-72-7	1000 g/L	400 g/L Soluble	EPI (2); Albright & Wilson, Ltd., 2000 (4), Rutgers Organics Corporation, 1997a (4)
	Xylene sulfonate, NH_4	26447-10-9	54 g/L	Soluble	EPI (2); Rutgers Organics Corporation, 1997b (4)
	Xylene sulfonate, Ca	28088-63-3	1000 g/L	553 g/L	EPI (2), Ruetgers-Nease Chemical, Inc., 1997c
	Cumene sulfonate, Na	28348-53-0	635 g/L	330 g/L , 400 g/L Soluble	EPI (2), Albright & Wilson Americas Inc., 1997 (4);, Huels AG, 1995a (4); Rutgers Organics Corporation, 1997c (4)
	Cumene sulfonate, NH_4	37475-88-0	22 g/L	-	EPI (2)
	Xylene sulfonate, K	30346-73-7	1000 g/L	-	EPI (2)

	Toluene sulfonate, K	16106-44-8	1000 g/L	-	EPI (2)
Partition coefficient n-octanol /water	Xylene sulfonate, Na	1300-72-7	log Kow = -1.86	-	EPI (2)
	Xylene sulfonate, Ca	28088-63-3	log Kow = -1.92	log Kow = -2.7	Ruetgers-Nease Chemical, Inc. 1997b
	Toluene sulfonate, Na	12068-03-0	log Kow = -2.4	-	EPI (2)
	Cumene sulfonate, Na	28348-53-0	log Kow = -1.5	-	EPI (2)
	Xylene sulfonate, NH_4	26447-10-9	log Kow = -0.13	-	EPI (2)
	Cumene sulfonate, NH_4	37475-88-0	log Kow = 0.23	-	EPI (2)
	Xylene sulfonate, K	30346-73-7	log Kow = -1.86	-	EPI (2)
	Toluene sulfonate, K	16106-44-8	log Kow = -2.4	-	EPI (2)

[1] The Klimisch reliability ratings are in parenthesis. A Klimisch reliability score of 1 = reliable without restrictions, 2 = reliable with restrictions, 3 = not reliable, 4 = not assignable. The modelled values (reference identified as "EPI") are based on EPIWIN and are assigned a reliability rating of 2. NOTE: "Pa" is Pascal.

2 GENERAL INFORMATION ON EXPOSURE

2.1 Production Volumes and Use Pattern

Approximately 29,000 metric tonnes of hydrotropes are introduced (i.e. manufactured and imported) annually to the U.S. (based on 2002 data). Annual production in Australia and Europe is approximately 1100 (40% concentration) and 19,000 tonnes, respectively (based on 2002 data). Hydrotropes are used at active concentrations between 0.1 and 15% in consumer cleaning and personal care products. There are no industrial process intermediate uses of the hydrotropes. Hydrotropes function as coupling agents in the following products:

Table 3. Concentrations of Hydrotropes in Products in the U.S. and Australia

Product Type	**Concentration in Products In U.S. (range)**	**Concentration in Products in Australia (range)**
laundry detergents		– 1.375%
powders	0.1 – 0.5 %	
liquids	1 – 10 %	
hard surface cleaners, including dilutable forms	– 5.0 %	– 0.9%
machine dishwashing rinse aid	1 – 5%	– 5.5%
hand dishwashing liquid detergents	1 – 5 %	1.2 – 5.5%
body washes	– 0.5 %	-
shampoo	1 – 5 %	– 0.8%
hair conditioner	1 – 5 %	-
face and hand soap (liquid)	10 – 15 %	-
toilet treatments	-	0.2%
solvent hand cleaner	-	0.8%
carpet cleaners	-	1%
optical brightener product	-	3%

Concentrations were calculated on a w/w basis.

In Australia, a relatively small volume (about 55 tonnes per year) is used in liquid sulphur textile dyes present at 7.5 – 50%, acidic recirculation cleaning products present at 10-25%, wetting agent for tanning industry present at 10%, enzymatic recirculation cleaner for dairy and food processing

applications at 4%, coolant system conditioner at 6.9%, car wash detergents at 1.3–6.3%, cleaners and degreasers at 0.1–6.3%, vinyl, plastic rubber restorer at 0.2% and floor stripper at 2.7–9%.

2.2 Environmental Exposure and Fate

Based on its use pattern, the predominant disposal route following use of the products that contain hydrotropes is via wastewater. Hydrotropes are water soluble (>1000 mg/L) and have low volatility (vapour pressure between 1.1 x 10^{-9} to 3.56 x 10^{-7} Pa). Hydrotropes are rapidly and completely biodegraded and are effectively removed during biological wastewater treatment (~94%). It has low potential for bioaccumulation (estimated Bioconcentration Factor [BCF] approximately 3 L/kg). These characteristics help to minimize the potential for environmental exposure, and for indirect human exposure via drinking water and/or fish consumption.

2.2.1 Sources of Environmental Exposure

Releases to the Environment from Manufacturing and Formulation Processes:

Manufacturing and formulation processes have been designed to maximize production yield and minimize potential environmental releases. A limited amount of hydrotropes may be released as a dilute aqueous solution from washing and rinsing operations in the manufacturing and formulation processes. Atmospheric emissions are considered to be very low. Any minimal release from manufacturing that produce or formulate hydrotropes is discharged to wastewater treatment. Modelling of manufacturing facility effluent discharges using the U.S.EPA Exposure & Fate Assessment Screening Tool (E-FAST) for high end to bounding condition are provided in Annex 2.

Releases to the Environment Following Consumer Use:

Hydrotropes are used primarily in personal care and household/professional cleaning products. Environmental releases from down-the-drain discharges following product use could lead to potential ecological exposure in surface water. These hydrotropes are readily soluble (>1000 mg/L), have low volatility, and are predicted to partition almost completely to the water compartment. Products containing hydrotropes disposed of down-the-drain are transported to wastewater treatment plants where significant removal is expected. Residual hydrotropes entering the environment are expected to be completely biodegraded (>80% in ≤ 28 days in standard tests). They have a low potential for bioaccumulation (BCF <2.3) based on test results. These characteristics help to minimize the potential for long-term environmental exposure.

U.S. modelling (using U.S.EPA E-FAST) results of wastewater treatment plant discharges following down the drain disposal of consumer products for high end to bounding conditions are provided in Annex 2. There are no monitoring data available to compare to modelled estimations.

Australia modelling results of wastewater treatment plant discharges to rivers and oceans following down the drain disposal of consumer products for high end conditions are provided in Annex 2. There are no monitoring data available to compare to modelled estimations. Negligible partitioning to sewage sludge, and hence negligible exposure to agricultural soil, is expected.

2.2.2 Photodegradation

No experimental data are available for photodegradation of hydrotropes. Photodegradation rates were estimated for cumene sulfonate (40 hours), xylene sulfonates (41 hours) and toluene sulfonates (105 hours) using AOPWIN™ (in EPIWIN 3.11). The predicted atmospheric oxidation

half lives indicate a significant atmospheric degradation potential (Health and Environmental Safety Alliance, 2003). Input parameters were those listed in Table 2 for vapour pressure, boiling point, melting point and octanol water partition coefficient. Note that hydrotropes are not volatile, which reduces the importance of atmospheric photodegradation as an environmental fate mechanism, therefore no further consideration is given to this compartment in the assessment.

2.2.3 Stability in Water

No measured data are available for hydrolysis of the hydrotropes category; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

2.2.4 Transport between Environmental Compartments

Fugacity modelling has been conducted to determine the theoretical distribution of hydrotropes in various environmental compartments. Based on EQC Level III modelling, the key compartment for fate of hydrotropes will be surface waters, with a predicted partitioning of 99.9% (Health and Environmental Safety Alliance, 2003). The EQC Model is a widely used and accepted screening methodology; descriptions, applications and the model itself are available from the Canadian Environmental Modeling Centre (Trent University) at http://www.trentu.ca/cemc/welcome.html and from the U.S.EPA at http://www.epa.gov/opptintr/exposure/docs/hpvscn.htm.

Table 4 presents the output summary for two hydrotropes. First is calcium xylene sulfonate, which is based upon measured physico-chemical property data for all the input parameters except for vapour pressure. Second is sodium cumene sulfonate, which has the lowest estimated water solubility reported among the hydrotropes category and therefore would be expected to represent a hydrotrope with the lowest partitioning to water. The modelled physico-chemical input parameters for sodium cumene sulfonate are derived using EPIWIN. Modelled partitioning is nearly identical for both chemicals. Similar partitioning behavior would be expected across the range of hydrotropes category independent of the benzene substitution (i.e., toluene, xylene or cumene) and counter ion (i.e., Na, K, NH_4, Ca). Hydrotropes are predicted to reside 99+% in the water fraction.

Table 4: EQC model output

Calcium Xylene Sulfonate (top row) and Sodium Cumene Sulfonate (bottom row)

MW	Water Solubility (mg/L)	Octanol-Water Partition Coefficient (Log Kow)	Melting Point (°C)	Vapour Pressure (Pa)	Fraction in Soil (%)	Fraction in Air (%)	Fraction in Water (%)	Fraction in Sediment (%)
226	553 000	-2.7	375	1.2×10^{-11}	0.1	Negligible	99.9	Negligible
222	330 000	-1.5	300	1.09×10^{-9}	0.1	Negligible	99.9	Negligible

Emission level used for level III modelling was 3310.5 kg/h to water (calculated based on 29,000 tonnes released over 365 days, 24 hours per day); Emission levels used for level II modeling was the default 1000 kg/h to water. Outputs for level II and III are almost identical.

2.2.5 Biodegradation

Hydrotropes are fully biodegradable under aerobic conditions. Studies with toluene, xylene and cumene sulfonates are available and are summarized in Table 5. As a group, the hydrotropes category is considered as readily biodegradable according to OECD criteria. The two reports of MITI test results indicate no biodegradation in 28 days. This result is totally inconsistent with that for the remaining 11 tests which include ready biodegradation and inherent biodegradation studies using OECD protocols. No data are available on anaerobic degradation.

Table 5: Aerobic Biodegradation Screening Tests on Hydrotropes

Ready Biodegradation Results

Compound	CAS No.	Ready Aerobic Biodegradation	Method	Reference[1]
Toluene sulfonate, Na	12068-03-0	0% in 28 days	MITI Test, OECD301C	CERI, 1996d (2)
Xylene sulfonate, Na	1300-72-7	74% degraded in 15 days, 88% in 28 days	Modified Sturm; OECD301B	Stepan Company, 1993 (2)
Xylene sulfonate, Na	1300-72-7	74% degraded in 15 days, 84% in 28 days	Modified Sturm, OECD301B	Ruetgers-Nease Chemical, 1992c (1) CERI, 1996c (2)
Xylene sulfonate, Na	827-21-4	0% in 28 days	MITI Test, OECD301C	
Xylene sulfonate, Ca	28088-63-3	>50% degraded in 15days, >80% in 29days	Modified Sturm, OECD301B	Ruetgers-Nease Chemical, 1994f (1)
Cumene sulfonate, Na	28348-53-0	>60% degraded in 6 days, 100% in 15 day	Modified Sturm, OECD301B	Ruetgers-Nease Chemical., 1993 (1) Greim et al., 1994 (4)
Cumene sulfonate, Na	28348-53-0	82.5-91.5% degraded (no duration given)	Coupled Unit, OECD301E	Huels AG, 1995a (4)
Cumene sulfonate, Na	28348-53-0	94% degraded (no duration given)	Modified Screen, OECD301E	

[1] The Klimisch reliability ratings are in parenthesis.

Inherent Biodegradation Results

Compound	CAS No.	Ready Aerobic Biodegradation	Method	Reference[1]
Cumene sulfonate, Na	28348-53-0	100% degraded (no duration given)	Zahn Wellens, OECD302B	Huels AG, 1995a (4)

[1] The Klimisch reliability ratings are in parenthesis.

Biodegradation Results from Non-Standard Tests

Compound	CAS No.	Ready Aerobic Biodegradation	Method	Reference[1]
Toluene sulfonate, Na	12068-03-0	100% after 3 days	Sewage inoculum	Continental Oil Company, 1965 (2)

Xylene sulfonate, Na Xylene sulfonate, NH_4	1300-72-7 26447-10-9	69% degraded in 5 days, 100% in 8 days 71% degraded in 26 days	Sewage inoculum Ultimate biodegradation	Continental Oil Company, 1965 (2) Procter & Gamble Company 1981 (4); The Soap and Detergent Association, 1973-1978 (4)
Cumene sulfonate, Na	28348-53-0	73% degraded (no duration given)	Not specified	The Soap and Detergent Association, 1973-1978 (4)

[1] The Klimisch reliability ratings are in parenthesis.

2.2.6 Bioaccumulation

There are two reported tests for fish bioaccumulation; sodium xylene sulfonate – CAS No. 827-21-4 (CERI, 1996e) and sodium toluene sulfonate – CAS 12068-03-0 (CERI, 1996f). Both tests were 42-day exposures of *Cyprinus sp.* following OECD guideline protocol 305C. The tests included two exposure concentrations (0.5 and 0.05 mg/L of sodium xylene sulfonate, and 0.001 and 0.0001 mg/L of sodium toluene sulfonate) in flow through systems. In both tests the measured BCF value was reported as less than 2.3. All measured values were lower than the detection limit of the HPLC analysis. The studies have a reliability rating of 2. BCFWIN predictions (Health and Environmental Safety Alliance, 2003) using the estimated log Kow value of –1.5 L/kg as input parameter (derived for sodium cumene sulfonate), calculated a bioconcentration factor of approximately 3 L/kg. Thus the potential for bioaccumulation of hydrotropes in aquatic organisms is predicted to be very low.

2.2.7 Other Information on Environmental Fate

Removal of hydrotropes from secondary activated sludge sewage treatment processes is greater than 94%, as observed in a modified SCAS study with calcium xylene sulfonate (Ruetgers-Nease Chemical, Inc., 1994). The protocol followed OECD Guideline 302A. The microbial inoculum was activated sludge mixed liquors from an operating municipal wastewater treatment plant. The concentration of hydrotrope tested was 20 mg carbon/L. The experimental design included duplicate test units, and 7 days each for sludge acclimation, for test substance acclimation, and for test substance removal measurements. The reliability rating for the study was 1. Monitoring data are not available for hydrotropes category.

2.3 Human Exposure

2.3.1 Occupational Exposure

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further

mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

No workplace air monitoring data are available. No occupational exposure limits (OELs) have been assigned for these chemicals.

2.3.2 Consumer Exposure

Hydrotropes are used in consumer/professional cleaning and personal care products, which may be used "as is", or diluted prior to or during use. Dermal contact will occur with these products. There is some potential for incidental or accidental ingestion of, inhalation of, and/or eye contact with products during handling and use. Exposure to hydrotropes in formulated consumer products is mitigated by following use and precaution instructions on product labels. Human exposure will be mitigated by the fact that residues from many of these products are washed or rinsed off. Results of dermal exposure modelling for use of products containing hydrotropes are reported in Annex 2. Environmental releases from production facilities and from down-the-drain discharges following product use may lead to potential environmental exposures in surface waters and indirect human exposures via drinking water and/or fish consumption. Results of indirect human exposure modelling combining both drinking water and fish consumption following both production facility and down-the-drain discharges is reported in Annex 2.

3 HUMAN HEALTH HAZARDS

3.1 Effects on Human Health

Data on all of the SIDS endpoints are available taking into account all the chemicals included in the hydrotropes category. Annex 1 Table B identifies the various endpoints and the available data.

3.1.1 Toxicokinetics, Metabolism and Distribution

No ADME (adsorption, distribution, metabolism and elimination) studies for the hydrotropes category were identified during this assessment. However, using the physico-chemical properties of the hydrotropes and available toxicological information a general qualitative comment can be made on absorption. The key physico-chemical properties available for undertaking such an evaluation are the molecular weight, water solubility and octanol/water partition coefficient (Log P) value. The molecular weight of these hydrotropes is 194-226 and a water solubility and Log P value of 553 g/L and –2.7 respectively are available (both from studies with xylene sulfonate calcium and with reliability ratings of 1).

Molecular weights below 500 are favourable for absorption from the gastrointestinal tract. Additionally, absorption of very hydrophilic substances, such as the hydrotropes, can occur by passive diffusions and if the molecular weight is low (less than 200) the substance may pass through aqueous pores. The observation of clinical signs of toxicity, such as decreased activity, weakness and prostration in the acute oral study supports the conclusion that, qualitatively, significant absorption occurs following oral administration of high doses.

In contrast to oral absorption, a molecular weight less than 100 favours dermal uptake. Additionally, if water solubility is above 10 g/L and the log P <0, as is the case for the hydrotropes, the substance is likely to be too hydrophilic to cross the lipid rich environment of the stratum corneum and dermal uptake of these substances will be low. The absence of clinical signs of

toxicity in the acute and repeat dermal toxicity studies support the conclusion that, qualitatively, limited absorption occurs following dermal administration.

Therefore, overall, the available data suggests that absorption will be significantly greater following oral exposure as compared to dermal.

3.1.2 Acute Toxicity

Studies in Animals

Table 6 provides the available acute toxicity results for toluene, xylene and cumene sulfonates and their various salts. Clinical signs observed in some of the acute oral toxicity studies included decreased activity, weakness, prostration, increased salivation, diarrhea, ptosis and anogenital staining. No clinical effects were reported following inhalation and dermal exposures. Necropsy findings reported in these same studies included slight pulmonary inflammation, gastrointestinal inflammation and hemorrhage, mild liver changes, congestion of liver, kidneys, adrenal glands and gastrointestinal tract, and redness of stomach mucosa in animals that died. Observations were within normal limits with a report of slight to moderate congestion of adrenal glands in animals that survived. Clinical signs observed in acute dermal exposure included erythmea with additional desquamation. At necropsy, findings reported were focal or multifocal red discoloration and desquamation of the treated skin. A number of the results are reported with limited study detail as part of summary reports. One-half of the oral studies and one dermal study are reported in considerable detail with regard to methods and results. Oral, dermal and inhalation acute toxicity endpoints are addressed. [Note that because purity information was not always available these acute toxicity data are not reported as "a.i." based on % active ingredient]

Table 6: Acute Mammalian Toxicity of Hydrotropes Category

Compound	CAS No.	Acute Toxicity Endpoints	Method	Reference[1]
Toluene sulfonate, Na	12068-03-0	Oral rat LD_{50} 6500 mg/kg bw	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Toluene sulfonate, K	16106-44-8	Oral rat LD_{50} 4400 mg/kg bw	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Toluene sulfonate, Na	12068-03-0	Inhalation rat LC_{50} >557,000 mg/ m^3*	US CPSC CFR1500.40	The Soap and Detergent Association, 1973-1978 (4); Witco Chemical Corporation, 1977 (4)
Xylene sulfonate, Na	1300-72-7	Oral rat LD50 >5000 mg/kg bw	Not Specified	The Soap and Detergent Association, 1973-1978 (4); Witco Chemical Corporation, 1977 (4)
Xylene sulfonate, Na	1300-72-7	Oral rat LD_{50} 7200 mg/kg bw	Not Specified	Albright & Wilson, Ltd., 2000 (2); Marchon Products Ltd., 1965 (2)
Xylene sulfonate, Na	1300-72-7	Oral rat LD_{50} 16,200 mg/kg bw	Not Specified	Continental Oil Company, 1975a (2)
Xylene sulfonate, Na	1300-72-7	Oral rat LD_{50} >5000-16,200 mg/kg bw	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Xylene sulfonate, NH_4	26447-10-9	Oral rat LD_{50} >2100 mg/kg bw	Not Specified	Unilever Research Laboratory, 1981 (4)
Xylene sulfonate, Ca	28088-63-3	Oral rat LD_{50} 3346 mg/kg bw	USEPA 798.1175	Ruetgers-Nease Chemical, Inc., 1994d (1)
Xylene sulfonate, Ca	28088-63-3	Dermal rabbit 24-hr LD_{50} >2000 mg/kg bw	USEPA 798.1100	Ruetgers-Nease Chemical, Inc., 1994b (1)
Xylene sulfonate, NH_4	26447-10-9	Inhalation rabbit 4-hr LC_{50} >6410 mg/m^3	Not Specified	Unilever Research Laboratory, 1981 (4)

Cumene sulfonate, Na	28348-53-0	Oral rat LD_{50} >7000 mg/kg bw	OECD 401	Greim et al., 1994 (4); Huels AG, 1995a (4); Huels AG, 1982a (2)
Cumene sulfonate, Na	28348-53-0	Dermal rabbit $L_{50}D$ >2000 mg/kg bw	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Cumene sulfonate, Na	28348-53-0	Inhalation rat LC_{50} >770,000 mg/ m^3*	US CPSC CFR1500.40	The Soap and Detergent Association, 1973-1978 (4); Witco Chemical Corporation, 1977 (4)

[1] The Klimisch reliability ratings are in parenthesis.
*USCPSC = U.S. Consumer Product Safety Commission CFR = Code of Federal Register (U.S.)

Conclusion

Across the hydrotropes category, the acute oral LD_{50} in rats ranges from 3346 mg/kg bw (1044 mg a.i./kg bw based on a 31.2% purity of the test substance) to 16,200 mg/kg bw (6480 mg a.i./kg bw based on a 40% purity of the test substance) and, the dermal LD_{50} in rabbits is >2000 mg/kg bw (624 mg a.i./kg bw in a 24-hour exposure period based on a 31.2% purity of the test substance). The hydrotropes tested were of varying concentrations and the purity was not always reported which means toxicity based on active ingredient is not always available. Overall, hydrotropes demonstrate a relatively low order of acute oral and dermal toxicity. The results are consistent across the toluene, xylene and cumene sulfonates and their various salts. An acute inhalation study is available in the rabbit that suggests low acute toxicity for ammonium xylene sulfonate (LC50 > 6,410 mg/m^3/4 hr). However only minimal data was available for this study and the reliability rating of this study is 4. Acute inhalation studies in rats at much higher levels (> 500,000 mg/m^3) are also available for sodium toluene sulfonate and sodium cumene sulfonate. The duration of exposure was not provided, however no toxicity was observed.

3.1.3 Irritation

Tables 7 and 8 provide the available skin and eye irritation results for toluene, xylene and cumene sulfonates and their various salts. A number of the results are reported with limited study detail as part of summary reports; however, several studies include considerable detail with regard to methods and results.

Table 7: Skin Irritation Studies of Hydrotropes Category

Compound	CAS No.	Irritation Endpoints	Exposure Duration/Dose	Method	Reference[1]
Toluene + xylene sulfonates, Na [50:50]	12068-03-0 + 1300-72-7	Mild to moderate irritation to rabbit skin with 40% solution	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Xylene sulfonate, Na	1300-72-7	Slight irritation to rabbit skin with 40% solution	24hrs / 0.5ml	Not Specified	Continental Oil Company, 1975b (2)
Xylene sulfonate, Na	1300-72-7	Slight irritation to rabbit skin with 40% solution	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4); Unilever Research Laboratory, 1981 (4)
Xylene sulfonate, NH_4	26447-10-9	Slight irritation to rabbit skin. (concentration not indicated)	Not Specified	Not Specified	Unilever Research Laboratory, 1981 (4)

Xylene sulfonate, Ca	28088-63-3	Not irritating to rabbit skin. Purity of the test material-31.2%	4hrs / 0.5ml	US EPA 81-5 & US EPA TSCA 798	Ruetgers-Nease Chemical, Inc, 1994j (1)
Cumene sulfonate, Na	28348-53-0	Not irritating to rabbit skin with 60% solution	4hrs / 0.5g	OECD 404	Huels AG, 1982c (2)
Cumene sulfonate, Na	28348-53-0	Mild to moderate irritation to rabbit skin. Test material- 1% active, undiluted.	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Cumene sulfonate, Na	28348-53-0	Not irritating to rabbit skin (concentration not indicated)	Not Specified	OECD 404	Huels AG, 1995a (4)
Cumene sulfonate, Na	28348-53-0	Not irritating to skin (concentration not indicated)	Not Specified	Not Specified	Greim et al., 1994 (4)

[1] The Klimisch reliability ratings are in parenthesis.
TSCA = Toxic Substances Control Act (U.S.)

Table 8: Eye Irritation Studies of Hydrotropes Category

Compound	CAS No.	Irritation Endpoints	Exposure Duration /Dose	Methods	Reference
Toluene sulfonate, Na	12068-03-0	Moderate irritation to rabbit eye with 20% solution	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Toluene sulfonate, K	16106-44-8	Slight irritation to rinsed and non rinsed rabbit eye with 20% solution. Irritation with rinsed 50% solution	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Xylene sulfonate, Na	1300-72-7	Slight irritation to rabbit eye with 40% solution	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4); Unilever Research Laboratory, 1981 (4); Witco Chemical Corporation, 1977 (4)
Xylene sulfonate, NH_4	26447-10-9	Slight irritation to rabbit eye (concentration not indicated)	Not Specified	Not Specified	Unilever Research Laboratory, 1981 (4)
Xylene sulfonate, Ca	28088-63-3	Mild irritation to rabbit eye. Purity of test material-31.2%	0.1ml	US EPA TSCA 798.4500	Ruetgers-Nease Chemical, Inc., 1994k (1)
Cumene sulfonate, Na	28348-53-0	Irritating to rabbit eye depending on diluted or not, and rinsed or not at 10% solution	Not Specified	Not Specified	The Soap and Detergent Association, 1973-1978 (4)
Cumene sulfonate, Na	28348-53-0	Not irritating to rabbit eye (concentration not indicated)	Not Specified	Not Specified	Greim et al., 1994 (4)
Cumene sulfonate, Na	28348-53-0	Not irritating to rabbit eye	Not Specified	OECD 405	Huels AG, 1995a

		(concentration not indicated)			(4)
Cumene sulfonate, Na	28348-53-0	Mild irritation to rabbit eye with 60% solution, 96% purity of test substance	50mg	OECD405	Huels AG, 1982b (2)

[1] The Klimisch reliability ratings are in parenthesis.

Conclusion

A series of rabbit skin and eye irritation studies are reported for members of the hydrotropes category. Sodium xylene sulfonate is not a skin irritant. Calcium xylene sulfonate and sodium cumene sulfonate are not skin irritants and both caused slight but reversible eye irritation.

3.1.4 Sensitization

Studies in Humans

Skin

In the only available study, no evidence of skin sensitization was reported in a human repeat insult patch test of 0.5% aqueous sodium cumene sulfonate in a 0.1 % aqueous solution of granular laundry detergent product (The Soap and Detergent Association, 1973-1978). However, the available information does not allow the reliability of the study to be determined (reliability rating of 4)

Studies in Animals

A guideline study with guinea pigs reports no evidence of skin sensitization following dermal, occlusive exposure to a 42.8% solution (deionized water) of sodium toluene sulfonate (Hüls AG, 1995b). No irritation was observed during the entire study (neither at induction nor at challenge). The protocol follows the Buehler Test and the reliability rating of this GLP study is 1.

Conclusion

There is no indication of skin sensitisation potential for the hydrotropes category based on the available animal study (GLP Buehler test). No reliable human data are available.

3.1.5 Repeated Dose Toxicity

Oral and dermal subchronic repeat dose toxicity studies conducted in rats and mice are available for the hydrotropes category. The results are summarized in Table 9.

Studies in Animals

Dermal

Two subchronic dermal toxicity studies in both rats and mice were conducted using technical grade sodium xylenesulfonate (65% purity of test substance) in water (in 17-day) and ethanol (in 90-day) vehicles (NIH, 1998). All four studies are detailed in a 1998 U.S. National Institutes of Health report and have been assigned a reliability rating of 2. Five doses and a vehicle only were applied 5 days per week to clipped skin. In the 17-day study, doses ranged from 10-800 mg active ingredient (a.i.)/kg body weight (bw) for male rats, 13-1030 for female rats, 20-1600 for male mice and 26-2000 mg a.i./kg bw for female mice. In the 90-day study, doses ranged from 6-500 mg a.i./kg bw for male rats, 10-800 for female rats, 17-1300 for male mice, and 20-1620 for female mice. The 17-day study exposed 5 animals per sex per dose and the 90-day study exposed 10 animals per sex per

dose. Rats were 5-6 weeks old and mice were 6-7 weeks old at study initiation. Endpoints in the 17-day study were mortality, body and organ weight, clinical signs and histopathology of skin from site of application, skin from an untreated site, and gross lesions. Endpoints in the 90-day study were the same as 17-days but also included hematology, clinical biochemistry and complete histopathology at necropsy on control mice and rats as well as on top dose group (1620 mg a.i/kg bw/day in females and 1300 mg a.i./kg bw/day) males. No treatment-related deaths occurred in either study.

No treatment related effects were observed in the 17-day study for either species. The highest doses were 2000 mg a.i./kg bw for mice and 1030 mg a.i./kg bw for rats. The relative liver weights of male and female rats at the two highest doses were significantly greater than those of the control groups but the absolute weights were similar. The biological significance of the differences in relative liver weights was unclear. Similar observations and conclusions were reported in the mouse study at all the doses for males and at the highest dose for females.

No treatment related effects were observed in the 90-day study for rats. The highest dose was 800 mg a.i./kg bw in females and 500 mg a.i./kg bw in males. The absolute and relative liver weights of males at the mid (60 and 170 mg a.i./kg bw) and upper (500 mg a.i./kg bw) doses were significantly less than those of the controls. A dose response effect was not observed at the three doses. There were no treatment-related histopathologic alterations in the livers, thus the biological significance of the decreased liver weights was unclear.

No treatment related effects were observed in the 90-day study for female mice at the highest dose which was 1620 mg a.i./kg bw. There was however, a gain in mean body weight and kidney weight in male mice at the highest dose of 1300 mg a.i./kg bw. The gain in body weight though statistically significant was <10% of the controls and is not considered to be toxicologically significant. There were no clinical findings related to sodium xylene sulfonate administration. There was some epidermal hyperplasia (reported as “typically minimal in severity” multifocal increase in the thickness of the epidermis) observed in male and female mice at the highest doses. However, the results of the 2-year study (NIH, 1998) conducted by the same investigators (reported below) showed no evidence that these lesions progressed to skin neoplasms. The No Observed Adverse Effect Level (NOAEL) for local effects, based on epidermal hyperplasia at the site of application, was 440 mg a.i./kg bw for male mice and 540 mg a.i./kg bw for female mice.

Oral

Three subchronic 90-day feeding studies in rats were conducted; two with sodium xylene sulfonate (Albright & Wilson Ltd., 1969; Tracor Jitco, Inc., 1980) and the other with sodium cumene sulfonate (Procter & Gamble Company, 1968). One of the studies also included mice (Tracor Jitco, Inc., 1980).

In the first study (Albright & Wilson Ltd., 1969), 15 Wistar rats per sex per dose level were exposed to purified sodium xylene sulfonate at 0, 0.2, 1.0 and 5.0% in the diet. Mean administered doses were 0, 140, 710 and 3800 mg/kg bw for males and 0, 160, 820 and 4400 mg/kg bw for females. The purity of the test substance was stated as at least 93% (Albright & Wilson, Ltd., 2000). Therefore, the doses based on active ingredient (a.i.) are 130, 660 and 3534 mg a.i./kg bw for males and 149, 763 and 4092 mg a.i./kg bw for females. Endpoints were those specified in OECD 408 with the exception of clinical signs, functional observations, ophthalmoscopy, cholesterol, sodium and potassium as part of clinical chemistry and platelets and blood clotting potential as part of hematology. The following organs were examined for histopathological changes: hearts, spleen, liver, kidney, brain, testicle/ovary, thymus, pituitary, thyroid and adrenal. No treatment related effects other than some sporadic clinical chemistry and haematology changes were observed in

males at up to the highest dose (3534 mg a.i./kg bw). A loss of relative spleen weight in females, along with some clinical chemistry and haematology changes, was observed at the highest dose (4092 mg a.i./kg bw). No treatment related histopathological changes were reported in the spleen or any other organ examined. The NOAEL from this study is 1% or 763 mg a.i./kg bw in females and 5 % or 3534 a.i. mg/kg bw in males.

In the second study (Tracor Jitco, Inc., 1980), ten male and ten female Fischer rats and B6C3F1 hybrid mice were exposed per dose level to sodium xylene sulfonate at 0, 0.125%, 0.25%, 0.5%, 1% and 2% in the diet over a 91-day period. A nuclear magnetic resonance spectrum was run on the test material to determine purity. The conclusion of this analysis was that the major component of the test material was xylene sulfonate although an exact percent purity was not stated in the report. These dietary levels equate to 0, 152, 305, 610, 1220 and 2439 mg/kg bw daily doses for male mice, 0, 154, 308, 617, 1234 and 2467 mg/kg bw for female mice, 0, 89, 179, 357, 715 and 1429 mg/kg bw for male rats, and 0, 98, 195, 390, 781 and 1561 mg/kg bw for female rats. Body weights and food consumption were recorded. Animals were observed for clinical signs and mortality. No haematology or clinical chemistry tests were undertaken. Gross pathology was recorded when observed and histopathology was performed on all controls and high dose animals. There were no significant dose-related treatment effects on food consumption or body weight in any group for either species. There were also no treatment-related gross or microscopic lesions noted at necropsy in either rats or mice. The NOAELs therefore, are 2439 and 2467 mg/kg bw/day for male and female mice respectively and 1429 and 1561 mg/kg bw/day for male and female rats respectively.

In the third study (Procter & Gamble Company, 1968), 20 CD rats per sex per dose level were exposed to sodium cumene sulfonate at 0, 0.005, 0.05 and 0.5% in the diet. Mean administered doses were 0, 2.6, 26 and 270 mg/kg bw for males and 0, 3.6, 36 and 375 mg/kg bw for females. Taking into account the content of active ingredient, 42.3%, these doses equate to 1.1, 11 and 114 mg a.i./kg bw and 1.5, 15 and 159 mg a.i./kg bw, respectively. The intervals between dose levels are large (factor of 10), while OECD TG 408 prefers 2 – 4 fold intervals and an additional group if factors are > 6 – 10. Endpoints were mortality, body and organ weight, food consumption, haematology, and histopathology. The methodology of this study was not available for assessment and was deduced from the results provided. No treatment related effects were observed in males at up to the highest dose (114 mg a.i./kg bw). A reduction in body weight gain was reported in females (4%, 5% 12% as compared to controls at 1.5, 15 and 159 mg a.i./kg bw, respectively). The study report stated that this decrease in body weight gain was within the established ranges for animals of this species and age and was therefore not considered an adverse effect by the authors. The feed efficiency of the high dose females was statistically higher than the controls. The decrease in body weight gain of the high dose females was not associated with histopathological changes or any other effects. Histopathological studies indicated that severe tubule atrophy and degeneration had occurred in the testes of one animal treated at the highest dose. Similar but a mild lesion was seen in one male treated with 15 mg a.i./kg bw, test substance. Histopathological confirmation study took tissues from 4 additional controls rats and 12 treated rats (presumably 4 males from each dose). No lesions attributable to the treatment were evident. Prostatitis was observed in two animals in the lowest dose group, but no dose response effect was seen. The authors stated that there was also a slight increase in the number of animals with the pulmonary lesions common to the rat (i.e. perivasculitis and peribronchitis), however, there was no difference in the incidence between the control and treated rats. Of the 16 rats that were used for the histopathology confirmation study 11 had murine pneumonia (no differentiation was made between the controls and treated). The NOAEL for sodium cumene sulfonate is therefore 114 mg a.i./kg bw for males and 159 mg a.i./kg bw for females.

Two 14 day studies in rats (Tracor Jitco, Inc., 1979, Tracor Jitco, Inc., 1980b) and one (Tracor Jitco, Inc., 1979) in mice are available for sodium xylene sulfonate. One of the studies was a two-week range-finding study in both mice and rats (Tracor Jitco, Inc., 1979) and preceded a 90-day study (Tracor Jitco, Inc., 1980a) described above. The dose concentrations in this study were 0, 0.25, 0.5, 1, 2% and 4%. Body weight and food consumption were recorded and the animals were observed for clinical signs and mortality. There were no clinical signs of toxicity or mortality at any of the doses in mice. Body weight gain was higher than the controls at the 0.25 and 0.5% levels in both sexes of mice. At 1, 2 and 4% levels the body weight gain was reduced by 2, 2 and 6% of control values, respectively. Reduced weight gain at the higher dose levels may be related to feed consumption which was slightly decreased in the first week with an increase in feed consumption in the second week. This could be the result of a palatability issue with acceptability of the feed in the second week in mice. Animals were observed scratching the food out of their dishes beginning about day 5.

In rats, deaths occurred at 2% (2 animals) and 4% (4 animals) in males, and in females one each at the 0.5, 1, 2 and 4% doses. The deaths in males occurred on days 7, 8 and 12. Body weight gains were reduced by 3 and 19% of the control value at 1 and 2% levels in males, respectively. At the 4% level in females body weight gain was reduced by 7% of the control value. Food consumption was generally higher in the second week. Palatability was reported to be a problem as many animals were scratching the feed out of the dish, developed rough coats, loss of weight followed by death of some of the animals.

Subsequent to the 90-day study (Tracor Jitco, Inc., 1980a), a second two-week study (Tracor Jitco, Inc., 1980b) was conducted because of the lack of toxicity noted in the subchronic study (Tracor Jitco, Inc., 1980a) and in light of the mortalities reported in the first two-week range-finding study (Tracor Jitco, Inc., 1979). This study was to determine if the mortalities observed in the first 14 day study were reproducible and related to the toxicity of sodium xylene sulfonate. The dose concentrations in this study were 0, 1, 2, and 4%. No mortality was observed at any dose levels. Reduced body weight gains were reported at 1, 2 and 4% doses in both sexes (5, 4 and 17% reductions as compared to control values in males, and 2, 2 and 5% reductions as compared to control values in females, respectively), however, there was no dose-response relationship between test material concentration and body weight gain. Palatability appeared to be an issue in the 4% group as animals were observed scratching their feed from the feeders during the last eight days of the study at this level. An accurate measurement of food consumption was not possible because of the food spillage issues.

Table 9 provides the available repeated dose toxicity studies for the hydrotrope category.

Table 9: Summary of Repeat Dose Toxicity Tests of the Hydrotropes Category

Compound	CAS No.	Species	Route of Exposure	Study Duration	NOAEL mg/kg bw	LOAEL mg/kg bw	Doses mg/kg bw	Reference[1]
Xylene sulfonate,Na	1300-72-7	Rat	Dermal	17-day	No effects at high dose (1030)	N/A	♂ 10, 30, 90, 260, 800 a.i. ♀ 13, 40, 120, 330, 1030 a.i.	NIH, 1998 (2)

Xylene sulfonate, Na	1300-72-7	Mouse	Dermal	17-day	No effects at high dose (2000)	N/A	♂ 20, 60, 190, 540, 1600 a.i. ♀ 26, 80, 220, 680, 2000 a.i.	NIH, 1998 (2)
Xylene sulfonate, Na	1300-72-7	Rat	Dermal	90-day	No effects at high dose (800)	N/A	♂ 6, 20, 60, 170, 500 a.i. ♀ 10, 30, 90, 260, 800 a.i.	NIH, 1998 (2)
Xylene sulfonate, Na	1300-72-7	Mouse	Dermal	90-day	540 for ♀ 440 for ♂	1620 for ♀ 1300 for ♂ epidermal hyperplasia	♂ 17, 50, 140, 440, 1300 a.i. ♀ 20, 60, 170, 540, 1620 a.i.	NIH, 1998 (2)
Xylene sulfonate, Na	1300-72-7	Mouse	Dermal	2-years	No systemic effects at high dose (727)	N/A	182, 364, 727 a.i.	NIH, 1998 (1)
Xylene sulfonate, Na	1300-72-7	Rat	Dermal	2-years	No systemic effects at high dose (240)	N/A	60, 150, 240 a.i.	NIH, 1998 (1)
Xylene sulfonate, Na	1300-72-7	Rat	Oral feed	14 days	Mortalities at 2, 4% levels. Palatability problem		0, 0.25, 0.5, 1, 2, 4% of diet	Tracor Jitco, Inc., 1979 (2)
Xylene sulfonate, Na	1300-72-7	Rat	Oral feed	14 days	No effects 4 %		0, 1, 2 and 4% of diet	Tracor Jitco, Inc., 1980b (2)
Xylene sulfonate, Na	1300-72-7	Mouse	Oral feed	14 days	No effects 4%		0, 0.25, 0.5, 1, 2, 4% of diet	Tracor Jitco, Inc., 1979 (2)
Xylene sulfonate, Na	1300-72-7	Rat	Oral feed	28-day	No effects 3% of diet	N/A	1% and 3% of diet	Albright & Wilson, Ltd., 2000 (4)
Xylene sulfonate, Na	1300-72-7	Rat	Oral feed	90-day	763 for ♀ No effects at high dose (3534) for ♂	4092 for ♀ relative spleen wt loss	♂ 130, 660, 3534 a.i. ♀ 149, 763, 4092 a.i.	Albright & Wilson, Ltd., 1969 (2)
Xylene sulfonate, Na	1300-72-7	Rat	Oral feed	90-day	No effects at high dose (1429 for ♂ 1561 for ♀)	N/A	♂ 89, 179, 357, 715, 1429 a.i. ♀ 98, 195, 390, 781, 1561 a.i.	Tracor Jitco, Inc., 1980a (2)
Xylene sulfonate, Na	1300-72-7	Mouse	Oral feed	90-day	No effects at high dose (2439 for ♂ 2467 for ♀	N/A	♂ 152, 305, 610, 1220, 2439 a.i. ♀ 154, 308, 617, 1234, 2467 a.i.	Tracor Jitco, Inc., 1980a (2)
Cumene sulfonate, Na	28348-53-0	Rat	Oral feed	91-day	No systemic effects at high dose (159)	N/A	♂ 1.1, 11, 114 a.i. ♀ 1.5, 15, 159 a.i.	Procter & Gamble 1968 (2)

[1] The Klimisch reliability ratings are in parenthesis.

Overall Conclusion:

The hydrotropes category has been assessed in repeated dose oral and dermal studies in rats and mice. Dermal studies have been conducted for up to 2 years at up to 727 mg a.i./kg bw. Oral studies have been conducted up to 90 days at up to 4092 mg a.i./kg bw. LOAELs ranged from 1300 mg a.i./kg bw/day in dermal studies to 4092 mg a.i./kg bw/day in oral studies. The corresponding NOAELs were 440 mg a.i./kg bw/day in dermal studies and 763 mg a.i./kg bw/day in oral studies. Local effects in the dermal study (mouse) were epidermal hyperplasia at the site of application. The only systemic effect observed was a body weight gain in males, but this change was not considered to be biologically significant.

One oral study reported a LOAEL of 4092 mg a.i./kg bw and a NOAEL of 763 mg a.i./kg bw. Effects observed were a decrease in spleen weight in females along with some clinical chemistry and hematology changes. No adverse effects were reported in males.

A reduction in body weight gain was reported in an oral study with sodium cumene sulfonate. Given that two other well reported 90 day studies did not report a reduction in body weight gain at much higher doses, the effect in the sodium cumene sulfonate study is considered questionable. The most appropriate NOAEL for systemic toxicity from mammalian toxicity studies was therefore determined to be 763 mg a.i./kg bw/day based on a reduction in relative spleen weight at the higher dose in female rats and some clinical chemistry and hematology changes.

3.1.6 Mutagenicity

The hydrotropes category has been assessed for mutagenic potential in a variety of *in vivo* and *in vitro* assays. Specifically, mouse micronucleus assays with calcium xylene sulfonate and sodium cumene sulfonate, an Ames assay, mouse lymphoma, sister chromatid exchange, and chromosome aberration assay with sodium xylene sulfonate, an Ames assay with calcium xylene sulfonate and an Ames assay with sodium cumene sulfonate. All studies have a reliability rating of 1.

In vitro Studies

Ames Assays: The mutagenic potential of sodium xylene sulfonate (NIH, 1998), calcium xylene sulfonate (Ruetgers-Nease Chemical, Inc., 1994a) and sodium cumene sulfonate (Henkel KgaA, 1984a), were tested up to 10,000, 5,000 and 2000 µg a.i./plate, respectively, in the bacterial reverse mutation (Ames) assay using S*almonella typhimurium* strains TA98, TA100, TA1535, TA1537 and TA1538 in the presence and absence of metabolic activation. There was no evidence of mutagenicity observed for any of the three compounds with and without metabolic activation. Positive controls for sodium xylene sulfonate and calcium xylene sulfonate were reported to give results that confirmed the validity of the test. The negative result for sodium xylene sulfonate is corroborated by an Albright & Wilson study (2000) reported in the IUCLID.

Mouse Lymphoma Test: Technical grade (65% a.i.) sodium xylene sulfonate was tested for mutagenicity potential in L5178Y mouse lymphoma cells up to 5000 µg/mL with and without metabolic activation using supplemented Fischer's medium and 2500 µg/mL without metabolic activation using DMSO (NIH, 1998). Test concentrations were reported to be selected based on cytotoxicity. There were two independent tests with duplicate cultures per treatment per test concentration. The exposure period was 4 hours with and without metabolic activation and the incubation period was 48 hours. There was no mutagenic activity without metabolic activation and an equivocal result was reported with activation. The result was considered equivocal because the significant increase in mutant colonies noted in the first trial with S9 was not repeated in the second trial. Positive results were seen at the highest doses where cytotoxicity was also reported.

Sister Chromatid Exchange (SCE) Test: Technical grade (65% a.i.) sodium xylene sulfonate was tested at 500 – 5000 µg/mL (should convert to active ingredient) in Chinese hamster ovary cells with and without metabolic activation (NIH, 1998). There were two independent tests with an exposure period of 2 hours with metabolic activation (plus 25.5 hours incubation time) and initially up to 25.5 hours without metabolic activation. However, cytotoxicity (cell cycle delay) was reported at 2513 – 5000 µg/mL without metabolic activity that was addressed by lengthening the exposure time to 32.5 hours to ensure a sufficient number of scorable (second-division metaphase) cells. No clastogenic activity was recorded with metabolic activation. A significant increase in SCEs was observed without metabolic activity but only at dose levels that were reported to produce cell cycle delay. Positive controls produced clear increases in SCEs.

Chromosome Aberration Test: Technical grade (65% a.i.) sodium xylene sulfonate was tested in Chinese hamster ovary cells with and without metabolic activation (NIH, 1998). Test concentrations were 2513, 3750 and 5000 µg/mL. Exposure with metabolic activation was 2 hours and 18 hours without metabolic activation. Cells were harvested at 12 and 18 hours with and without metabolic activation, respectively. There was no clastogenic activity with and without metabolic activation. Positive controls gave results that confirmed the validity of the test.

In vivo Studies

Three mouse micronucleus cytogenetic assays were reported. One study with calcium xylene sulfonate (Nuetgers-Nease Chemical, Inc., 1994i) used a single intra-peritoneal (i.p.) injection of 0, 145, 290 or 580 mg a.i./kg bw (5 per sex per dose). Doses were selected from a preliminary dose ranging study. Two oral (gavage) studies are available with sodium cumene sulfonate. One study (Huels AG, 1992) used a single administration of 0 or 4467 mg a.i./kg bw (5 per sex per dose) with the dose selected from a preliminary dose ranging study, and the other (9) total doses of 400, 2000 and 4000 mg a.i./kg bw delivered in two equal applications 24 hours apart (7 per sex per dose). One male and 1 female died at the top dose in this repeated dose study. Negative results were obtained in all three studies. In all 3 assays the positive controls gave results that confirmed the validity of the test.

Conclusion

No positive results were seen in *in vitro* or *in vivo* studies. Thus the available data indicate that the chemicals in the hydrotropes category do not have a genotoxic potential.

3.1.7 Carcinogenicity

Chronic toxicity/carcinogenicity data exist for the hydrotropes category for both rats and mice dermally exposed for 2 years (US Department of Health and Human Services, 1998). Both studies have reliability ratings of 1.

Dermal

F344/N rats (50 per sex per dose) and B6C3F1 mice (50 per sex per dose) received dermal application to clipped skin 5 days per week of technical grade sodium xylene sulfonate (65% a.i.) in 50 % ethanol in a 2-year carcinogenicity study. Doses in the rat study were 0, 60, 120 and 240 mg a.i./kg bw/day and 0, 182, 364 and 727 mg a.i./kg bw/day in the mouse study. Observations were as per OECD 453 Guideline with the exception of clinical signs recorded monthly, and no observations of food consumption (feeding was *ad libitum*), blood parameters, urinalysis and organ weights were undertaken. Stability of the test compound in ethanol was confirmed. Body weight gain was not affected by the exposures in either species. No treatment related effects were observed with the exception of epidermal hyperplasia at the application site in female rats at 120 and 240 mg

a.i./kg bw/day, in female mice at 0, 364 and 727 mg a.i./kg bw/day and in male mice at 364 and 727 mg a.i./kg bw/day. There was no evidence of carcinogenic activity.

Conclusion

Chronic toxicity/carcinogenicity data exist for the hydrotropes category for both rats and mice dermally exposed for 2 years. There was no evidence of a carcinogenic potential for the hydrotropes category in these dermal exposure studies. It is noted that there is limited dermal absorption of hydrotropes.

3.1.8 Toxicity for Reproduction

Developmental toxicity in rats was evaluated for calcium xylene sulfonate (Ruetgers-Nease Chemical, Inc., 1994g). No fertility studies are reported for the hydrotropes category. However, the 91-day oral rat feeding study with sodium cumene sulfonate (Procter & Gamble Company, 1968), the 90-day feeding study with sodium xylene sulfonate (Albright & Wilson Ltd., 1969) and the 90-day and 2-year dermal studies with sodium xylene sulfonate (NIH, 1998) included examination of sex organs of both sexes. No treatment related effects on reproductive organs were reported.

Developmental Toxicity

Calcium xylene sulfonate (31% a.i.) was administered via gavage to female rats (30 per dose) at 0, 150, 1500 or 3000 mg/kg bw in water on days 6 to 15 of gestation (Ruetgers-Nease Chemical, Inc., 1994g). EPA TSCA Guideline 1985 was followed, and the reliability rating of this study is 2. Clinical symptoms were noted daily from day 6 to 20. Body weight gain and food consumption were recorded on day 0, 6, 9, 12, 16 and 20. All females were macroscopically examined on day 20 (or on day of death). The uteri were removed, weighed and examined for number of corpora lutea, number of implantation sites and number and location of fetuses and resorptions. Fetuses were inspected on total number, sex, weight and external, visceral (one-half) and skeletal (one-half) defects.

Only one animal died during the study (mid-dose). No treatment related effects were observed. An increase in food intake observed at the highest dose was considered to be within ranges of biological variation for this species. The NOAEL for maternal and foetal toxicity was the highest dose tested; 3000 mg/kg bw/day that corresponds to 936 mg a.i./kg bw/day.

Conclusion

The hydrotropes category has been evaluated for the potential to cause developmental toxicity in rats. Based on the OECD guideline study with calcium xylene sulfonate, hydrotropes are not considered to be developmental toxicants. While a reproductive study is not available for the hydrotropes category, reproductive organs of both sexes were examined in 90-day oral and 90-day and 2-year dermal repeated dose studies. There is no evidence from these repeat dose studies to suggest that these chemicals would have an adverse effect on reproductive organs.

3.2 Initial Assessment for Human Health

Toxicological studies have been conducted with numerous members of the hydrotropes category. Data on all SIDS-endpoints are available. These data demonstrate consistent results and a relatively low toxicity for these compounds. The quality of data is variable and while some of these studies were conducted prior to the effective date for Good Laboratory Practices (GLPs) or were non-guideline, some studies are generally of good scientific quality, show consistent results and are acceptable to support the overall profile of the category.

The available acute toxicity data indicate that the hydrotropes category has a low hazard potential. These tests were conducted with varying concentrations of hydrotropes. Acute oral LD_{50} values for rats range from 3346 (1044 mg a.i./kg bw) – 16,200 mg /kg bw (6480 mg a.i./kg bw). Acute dermal LD_{50} value was >2000 mg/kg bw (624 mg a.i./kg bw following 24 hr exposure). No acute inhalation studies with reliability ratings of 1 or 2 are available; 3 studies with reliability ratings of 4 (insufficient detail) are reported.

In a series of studies in rabbits varying results were observed in the skin and eye irritation studies. Either slight or no skin irritation was observed with 31-60% solutions, and mild eye irritation with a 60% solution. The hydrotropes category is therefore considered to have a low skin and eye irritation potential. There is no indication of skin sensitization of the hydrotropes category based on the available animal (GLP Buehler test). No reliable human data are available.

In repeated dose exposure to hydrotropes via oral and dermal routes, no significant toxicity was observed in 9 of 14 studies. The NOAELs in the 9 studies ranged from 159 - 2467 mg a.i./kg bw. One dermal study (mouse) reported a LOAEL of 1300 mg a.i./kg bw and a NOAEL of 440 mg a.i./kg bw in males for local effects. Effects observed were epidermal hyperplasia at the site of application. The only systemic effect observed was a body weight gain in males, but this change was not considered to be biologically significant. One oral study reported a LOAEL of 4092 mg a.i./kg bw and a NOAEL of 763 mg a.i./kg bw. Effects observed were a decrease in spleen weight in females. No adverse effects were reported for males. A reduction in body weight gain (>10%) was reported in an oral study with sodium cumene sulfonate. Given that two other well reported 90 day studies did not report a reduction in body weight gain at much higher doses, the effect in the sodium cumene sulfonate study is considered not to be reliable and its finding is set aside in favour of the more robust studies. The most appropriate NOAEL for systemic toxicity from mammalian toxicity studies was therefore determined to be 763 mg a.i./kg bw/day based on a reduction in spleen weight in female rats. The most appropriate NOAEL for local effects was determined to be 440 mg a.i./kg/bw based on epidermal hyperplasia at the site of application (dermal exposure) in male mice. The results of a 2-year dermal study conducted by the same investigators showed no evidence that these lesions progressed to skin neoplasms.

No evidence of genotoxicity was seen in *in vitro* and *in vivo* assays. No evidence of carcinogenicity was seen in 2-year dermal studies in rats and mice.

No developmental effects or maternal toxicity were observed in a developmental toxicity study where female rats were gavaged with up to 936 mg a.i./kg bw/day of calcium xylene sulfonate.

While a reproductive study is not available for the hydrotropes, the 91-day oral rat feeding study with sodium cumene sulfonate, the 90-day feeding study with sodium xylene sulfonate and the 2-year dermal studies with sodium xylene sulfonate included examination of the reproductive organs of both sexes and there was no evidence to suggest that these chemicals produce reproductive effects.

The results are consistent across the toluene, xylene and cumene sulfonates and their various salts where comparative data are available (i.e., acute oral and dermal eye and skin irritation, repeated dose and genotoxicity).

4 HAZARDS TO THE ENVIRONMENT

4.1 Aquatic Effects

Reliable data are available on all SIDS-endpoints for selected members of the category and analogues. Annex 1 Table A identifies the various endpoints and the data available for them. The

data cover fish, invertebrates and algae for xylene sulfonate (sodium, ammonium and calcium salts) and cumene sulfonate (sodium salt). Chronic toxicity to *Daphnia magna* and bacterial toxicity was reported for sodium cumene sulfonate. While the toluene benzene derivative is not represented in the available data set, the xylene and cumene benzene representatives are represented. Results are consistent for the chemicals tested, providing confidence in the ability to read-across for other category members.

Acute Toxicity Test Results

Based on hazard data, acute toxicity is considered to be uniformly low across the category (Table 10). Green algae are considered the most sensitive species with EC_{50} values of 230-236 mg/L a.i. and No Observed Effect Concentrations (NOECs) of 31-75 mg a.i./L. when tested with the sodium and calcium salts of xylene sulfonic acid, respectively. Fish and invertebrates did not demonstrate acute sensitivity at concentrations tested (>318 mg a.i./L) of xylene and cumene sulfonates (ammonium, calcium and sodium salts). However some sublethal effects were noted in two of the studies at the higher concentrations and included surfacing, loss of equilibrium, swimming on the bottom of the tank, dark discoloration, labored respiration and quiescence in some fish.

Table 10: Acute Aquatic Toxicity of the Hydrotropes Category

Compound	CAS No.	Acute Toxicity Endpoint Species and Duration EC50 / LC50 (mg/L)[1]	Method	Reference[2]
		Fish		
Xylene sulfonate, Na	1300-72-7	Rainbow trout 96-hr LC50 >408 a.i.	EPA 797.1400	Stepan Company, 1993c (2)
Xylene sulfonate, Na	1300-72-7	Fathead minnow 96-hr LC50 >400 a.i.	EPA 797.1400	Ruetgers-Nease Chemical, Inc., 1992b (2)
Xylene sulfonate, NH_4	26447-10-9	Bluegill 96-hr LC50 = 1060	Not specified	Procter & Gamble Company, 1981 (4)
Xylene sulfonate, Ca	28088-63-3	Rainbow trout 96-hr LC50 >490 a.i.	EPA 797.1400 (flow through)	Ruetgers-Nease Chemical, Inc., 1992m (1)
		Invertebrate		
Xylene sulfonate, Na	1300-72-7	*Daphnia magna* 48-hr EC50 >408 a.i.	EPA 797-1300	Stepan Company, 1993b (2)
Xylene sulfonate, Na	1300-72-7	*Daphnia magna* 48-hr EC50 >400 a.i.	EPA 797-1300	Ruetgers-Nese Chemical, Inc., 1992d (2)
Xylene sulfonate, Na	1300-72-7	*Artemia sp.* 48-hr EC50 >400	Not specified	Albright & Wilson, Ltd., 2000 (4)
Xylene sulfonate, Ca	28088-63-3	*Daphnia magna* 48-hr EC50 >318 a.i.	EPA 797-1300 (flow through)	Ruetgers-Nease Chemical, Inc., 1994c (1)
		Algae		
Xylene sulfonate, Na	1300-72-7	*Selenastrum* 96-hr EC50 = 230 NOEC = 31	EPA 797.1050	Stepan Company, 1993a (2)
Xylene sulfonate, Ca	28088-63-3	*Selenastrum* 96-hr EC50 = 236 a.i. NOEC = 75 a.i.	EPA 797.1050	Ruetgers-Nease Chemical, Inc., 1994e (1)

		Fish			
Cumene sulfonate, Na	28348-53-0	Fathead minnow 96-hr	LC50 >450 a.i.	EPA 797.1400	Ruetgers-Nease Chemical, Inc., 1992e (2)
Cumene sulfonate, Na	28348-53-0	*Leuciscus idus* 48-hr	LC50 >1000	DIN 38412, T15	Greim et al., 1994 (4); Huels AG, 1995a (4)
		Invertebrate			
Cumene sulfonate, Na	28348-53-0	*Daphnia magna* 48-hr	EC50 >450 a.i.	EPA 797-1300	Ruetgers-Nease Chemical, Inc., 1992b (2)
Cumene sulfonate, Na	28348-53-0	*Daphnia magna* 24-hr	EC50 >1000	DIN 38412, T11	Huels AG, 1995a (4)
		Algae			
Cumene sulfonate, Na	28348-53-0	*Scenedesmus* 72-hr	EC50 >1000	Algenwachstums-hemmtest - UBA	Huels AG, 1995a (4)
		Bacteria			
Cumene sulfonate, Na	28348-53-0	*Pseudomonas putida* 48-hr	EC50 >16,000	Bringmann-Kuehn	Huels AG, 1995a (4)

[1] "a.i." indicates active ingredient for those studies where test substance purity was reported.
[2] The Klimisch reliability ratings are in parenthesis.
EC50 = Effect concentration for 50 percent of organisms tested.
LC50 = Lethal concentration for 50 percent of organisms tested.

Conclusion

The hydrotropes category demonstrates a low level of acute aquatic toxicity to fish, invertebrates, algae and bacteria.

Chronic Toxicity Test Results

A single chronic study is reported for *Daphnia magna*. [Note: the 96-hour algal toxicity tests reported in Table 10 may also be considered chronic results.] There are limited details of presumably the same study in both a journal article citation (Greim et al., 1994) and an IUCLID (sodium cumene sulfonate, CAS No. 28348-53-0, 18 Feb 2000)(Huels AG, 1995). Both references have reliability ratings of 4. The study is described as a 21-day exposure, with a reproduction endpoint following method "Verlaengerter Toxizitaetstest bei Daphnia magna nach UBA (1984 standard)", and with no analytical monitoring. The 21-day EC50 is reported as 154 mg/L and the NOEC is reported as >30 mg/L in Greim et al. (1994) and <30 mg/L in the IUCLID (Huels AG, 1995). The study sponsor does not have a full laboratory report but did indicate that "Testing was done in 1987 without formal GLP but that GLP certification of the laboratory was received in 1989/1990. Test substance concentrations were 30, 100 and 300 mg/L as active ingredient (with no analysis performed)." The sponsor also provided tables summarizing the number of parent animals and offspring during the course of the study. These tables are appended to Huels AG (1995) for the purpose of this SIAR. The tables show no significant test substance related mortality of parent animals over the 21-day exposure period. The average number of offspring produced per day was 43 in the controls, 38 at 30 mg/L, 29 at 100 mg/L and 13 at 300 mg/L. These equate to 88% of control, 67% of control and 30% of control at 30, 100 and 300 mg/L, respectively. There are insufficient data to establish a statistically derived NOEC. It is uncertain whether the 88% of control response is a significant reduction in the number of young produced, but the data in the table do indicate that the "NOEC >30 mg/L" as reported in Greim et al. (1994) appears to be in error. The NOEC could be = 30 mg/L or < 30 mg/L. A chronic NOEC of approximately 30 mg/L would be consistent with the lowest algal chronic NOEC value of 31 mg/L and would also be in the range of a predicted NOEC based on the daphnia acute LC50 value of >450 mg/L divided by 10 (i.e., >45 mg/L).

4.2 Terrestrial Effects

No terrestrial toxicity data are available for members of the hydrotropes category. Given the low potential for hydrotropes reaching the terrestrial compartment (EQC modelling results), the lack of persistence (ready biodegradability under aerobic conditions) or bioaccumulation (BCFWIN modelling results), and the low likelihood of these chemicals partitioning to soil (EQC modelling results), generation of data in this area is not considered necessary.

4.3 Other Environmental Effects

Results of a microbial toxicity test are reported for sodium cumene sulfonate. The 48-hr EC10 for the bacteria *Pseudomonas putida* exposed in a Bringmann-Kuehn-Test is reported as >16,000 mg/L (Huels AG, 1995).

4.4 Initial Assessment for the Environment

Effects assessment: Reliable ecotoxicity and environmental fate data are available on all SIDS-endpoints for selected members of the category. The toxicity data cover fish, invertebrates and algae and the consistency of results for the chemicals tested provides confidence in the ability to read-across for other category members. Relatively low level toxicity, ready biodegradation and low potential for bioaccumulation indicate that the hydrotropes category does not pose a significant environmental hazard. The suggested aquatic Predicted No Effect Concentration (PNEC) is 2.3 mg/L (2,300 µg/L) calculated as the lowest EC50 for three species (algae, fish, and daphnia) divided by the recommended assessment factor of 100. The lowest EC50 is 230 mg/L (algal toxicity; sodium xylene sulfonate) divided by 100 equals 2.3 mg/L. This PNEC is consistent with what would be predicted using the chronic daphnia NOEC divided by 10, or using the 96-hour algal NOEC as a chronic endpoint divided by 10.

5 RECOMMENDATIONS

Human Health: The chemicals in this category are of low priority for further work because of their low hazard profile.

Environmental: The chemicals in this category are of low priority for further work because of their low hazard profile.

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Witco Chemical Corporation, Paterson, New Jersey, USA. Letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data. SDAHT09.

ANNEX 1. MATRIX OF THE MEASURED DATA OF ACCEPTABLE QUALITY FOR SIDS ENDPOINTS

These tables provide a matrix of the measured physico-chemical and ecotoxicity data (A), and mammalian toxicity data (B) of acceptable quality available for the hydrotropes category.

Table A shows the number of studies with reliability rating 1 or 2 available for this category for the physico-chemicals properties and environmental end points. Supporting data, including studies with a reliability rating of 3 or 4, are not included here.

Table A. Measured data of acceptable quality for selected SIDS endpoints[@]:

Chemical Name	**CAS No.**		**Physico-Chemical**			**Environmental Fate**					**Ecotoxicity**		
		M.W.	Sol.	Log Kow	V.P.	Photo[+]	Stabil wat.[*]	Transp.[#]	Biodeg	Bioacc	Fish	Daph.	Algae
Toluene sulfonic acid, sodium salt	12068-03-0	194.18	-	-	-	-	-	-	Yes	Yes	-	-	-
Toluene sulfonic acid, potassium salt	16106-44-8	210.29	-	-	-	-	-	-	-	-	-	-	-
Xylene sulfonic acid, sodium salt	1300-72-7 827-21-4	208.21	-	-	Yes	-	-	-	Yes	Yes	Yes	Yes	Yes
Xylene sulfonic acid, ammonium salt	26447-10-9	203.24	-	-	-	-	-	-	-	-	-	-	-
Xylene sulfonic acid, potassium salt	30346-73-7	224.32	-	-	-	-	-	-	-	-	-	-	
Xylene sulfonic acid, calcium salt	28088-63-3	226.31	Yes	Yes	-	-	-	-	Yes	-	Yes	Yes	Yes
Cumene sulfonic acid, sodium salt	28348-53-0 32073-22-6	222.24	-	-	-	-	-	-	Yes	-	Yes	Yes	-
Cumene sulfonic acid, ammonium salt	37475-88-0	217.27	-	-	-	-	-	-	-	-	Yes	-	-

For data to be considered acceptable quality, it must be rated 1 or 2 on the Klimisch scale and is expressed as "Yes".

Abbreviations and footnotes

Sol, water solubility; LogKow, octanol:water partition; V.P., vapour pressure; Photo, photodegradation; Transp, transport between environmental compartments; Stabil.wat., stability in water; Transp., transport between environmental compartments; Biodeg, biodegradation; Bioacc., bioaccumulation; Daph., daphnia.

*Stability in water is not considered a relevant endpoint as commercial hydrotrope products are used in aqueous solutions to help solubilize otherwise water insoluble ingredients.

#Transport between environmental compartments are modelled for use in the SIAR. Modelling puts >99% of hydrotropes in the water compartment.

+Modeled photodegradation data are available.

- No data available

@Additional testing for all of the above endpoints is not considered necessary given the known high degree of water solubility, low volatility and ready biodegradability of hydrotropes.

Table B shows the number of studies of reliability rating 1 or 2 available for this category for the health hazard end points and that the data set is complete for these SIDS endpoints. Supporting data, including studies with a reliability rating of 3 or 4, are not included here.

Table B. Measured data of acceptable quality for selected SIDS endpoints:

Chemical Name	CAS No.	Toxicity Data										
		AO	AD	AI	SI	EI	SE	Rep.	Geno	Repro	Dev	Car
Toluene sulfonic acid, sodium salt	12068-03-0	-	-	-	-	-	Yes	-	-	-	-	-
Toluene sulfonic acid, potassium salt	16106-44-8	-	-	-	-	-	-	-	-	-	-	-
Xylene sulfonic acid, sodium salt	1300-72-7 827-21-4	Yes (2)	-	-	Yes	-	-	Yes (4)	Yes (3)	-	-	Yes (2)
Xylene sulfonic acid, ammonium salt	26447-10-9	-	-	-	-	-	-	-	-	-	-	-
Xylene sulfonic acid, potassium salt	30346-73-7	-	-	-	-	-	-	-	-	-	-	-
Xylene sulfonic acid, calcium salt	28088-63-3	Yes	Yes	-	Yes	Yes	-	-	Yes (2) #	-	Yes	-
Cumene sulfonic acid, sodium salt	28348-53-0 32073-22-6	Yes	-	-	Yes	Yes	-	Yes	Yes	-	-	-
Cumene sulfonic acid, ammonium salt	37475-88-0	-	-	-	-	-	-	-	-	-	-	-

For data to be considered acceptable quality, it must be rated 1 or 2 on the Klimisch scale and expressed as 'Yes" with number of studies in bracket.

Abbreviations and Footnotes

AO, acute oral; AD, acute dermal; AI, acute inhalation; SI, skin irritation; EI, eye irritation; SE, sensitisation; Rep, repeated dose toxicity; Geno, genotoxicity; Repro, reproductive toxicity; Dev, developmental toxicity; Car, carcinogenicity. # Substance identity not available from reports. - No data available

ANNEX 2: HYDROTROPES USE AND EXPOSURE INFORMATION

[Note: This annex has not been reviewed by the OECD member countries]

Purpose:

To provide high end to bounding estimates of the potential environmental and human exposure to hydrotropes from its manufacture and its use in consumer products in the United States (U.S.) to complement an OECD SIDS Programme review of this category.

Coverage:

The report covers manufacturing and professional and consumer use for hydrotropes in the United States (U.S.) and in Australia.

Synthesis of Key Assessment Results:

Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients in personal care and household/professional cleaning products. Hydrotropes are produced by sulfonation of aromatic hydrocarbon solvents (i.e., cumene, toluene, and xylene). The resulting aromatic sulfonic acid is neutralized utilizing the appropriate base (e.g., sodium hydroxide) to produce the sulfonate or hydrotrope. The category includes ammonium, calcium, potassium and sodium salts that are described by 10 CAS numbers (6 are ICCA-sponsored and have HPV status in one or more OECD regions; 4 are non-HPV status and are included as supporting chemicals in the category).

Approximately 29,000 metric tonnes of hydrotropes are produced annually in the U.S. Annual production in Australia and Europe is approximately 1,100 and 19,000 tonnes, respectively. Hydrotropes are used at active concentrations between 0.1 and 15% in consumer cleaning and personal care products. They function as coupling agents in liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products.

In Australia, a relatively small volume (about 55 tonnes per year) is used in liquid sulphur textile dyes present at 7.5 – 50%, acidic recirculation cleaning present at 10-25%, wetting agent for tanning industry present at 10%, enzymatic recirculation cleaner for dairy and food processing applications at 4%, coolant system conditioner at 6.9%, car wash detergents at 1.3–6.3%, cleaners and degreasers at 0.1–6.3%, vinyl, plastic rubber restorer at 0.2% and floor stripper at 2.7–9 %. There are no industrial process intermediate uses of the hydrotropes. The predominant disposal route following use of the products that contain hydrotropes is via wastewater.

Hydrotropes are water soluble (>1000 mg/L) and have low volatility (measured vp $<2.0 \times 10^{-5}$ Pa). Hydrotropes are rapidly and completely biodegraded and are effectively removed during biological wastewater treatment (~94%). It has low potential for bioaccumulation (measured BCF is <2.3). These characteristics help to minimize the potential for human and environmental exposure. Engineering controls (e.g., closed system operation, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities and industrial end uses such as textile dye mitigate worker exposures and no special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes.

The aquatic PNEC of hydrotropes is 2,300 µg/L. Aquatic life exposure occurs as a result of

process loss discharge at production facilities (Format C #1) and/or from down-the-drain discharge following private (consumer) use of laundry/cleaning and personal care products (Format C #2 for USA and C#3 for Australia). The down-the-drain scenario represents the major disposal route to the environment. E-FAST exposure modelling predicts upper-bound, in-stream concentrations of 286.9 µg/L for a hypothetical large production facility in the U.S. on a small stream under low flow (7Q10) conditions, 16.5 µg/L for a large production facility on a mid-size stream under low flow (7Q10) conditions, 0.63 µg/L for a wastewater treatment facility following down-the-drain consumer disposal into a small stream under low flow (7Q10) conditions, and 0.048 µg/L for a wastewater treatment facility following down-the-drain consumer disposal into a mid-size stream under average flow conditions. The U.S. conditions were specifically modelled due to the significant production and consumption in this geography. For Australia, the estimated concentration in surface waters is 8.3 µg/L in ocean water and 83 µg/L in rivers, assuming wide dispersive release over 365 days of the year.

The most appropriate NOAEL for systemic toxicity (oral exposure) from mammalian toxicity studies was therefore determined to be 763 mg a.i./kg bw/day based on a reduction in spleen weight in female rats. The most appropriate NOAEL for local effects was determined to be 440 mg a.i./kg/bw based on epidermal hyperplasia at the site of application (dermal exposure) in male mice. Modelled estimates of environmental concentrations leading to indirect human exposure from drinking water and fish consumption (Formats C#1 and C#2) range from 1.23×10^{-5} to 2.63×10^{-8} mg/kg bw/day. The highest estimated human exposures (Format C#4) are from residuals following personal care product use. They range from 0.02-0.14 mg/kg bw/day for shampoos and hair conditioners to 0.11- 0.17 mg/kg bw-day for liquid face and hand soaps. Exposure estimates for cleaning product use and residuals on clothing range from 0.01- 0.08 mg/kg bw-day. All exposure evaluations include conservative (protective) input assumptions (e.g. all modelled human exposures are conservative due to use of a default assumption of 100% absorption). However, the physico-chemical data and available toxicological data suggest that dermal absorption is likely to be minimal. Consequently, the contribution to total body burden arising from dermal exposure to personal care products will be significantly less than the reported exposure values.

In the particular case of hydrotropes, use of all the noted product categories by a single consumer is plausible. A conservative estimate of aggregate daily exposure could be achieved by a simple addition of the daily exposure estimates for each of the product categories plus exposure estimates for drinking water and fish consumption. However, as stated, the body burden from dermal exposure will be significantly over-estimated and hence the margin of exposure between the calculated body burden and NOAEL would be considerably greater.

Identity of Organization

Hydrotropes Consortium
The Soap and Detergent Association, c/o Kathleen Stanton (kstanton@sdahq.org)
1500 K St. NW, Suite 300, Washington, DC 20005

Table of Contents

Format A: General Information

I. Substance Information

(1) Category Name:
Hydrotropes Category

(2) Substance Name(s) and CAS Numbers:
Hydrotropes are classified into one category and include the following ICCA-sponsored HPV CAS numbers and corresponding chemical names:

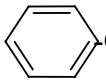
1300-72-7	xylenesulfonic acid, sodium salt
26447-10-9	xylenesulfonic acid, ammonium salt
12068-03-0	toluenesulfonic acid, sodium salt
28348-53-0	cumenesulfonic acid, sodium salt
32073-22-6	cumenesulfonic acid, sodium salt
37475-88-0	cumenesulfonic acid, ammonium salt

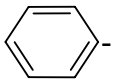
In addition, four CAS numbers that are not HPV hydrotropes and are not ICCA sponsored but are among the hydrotropes reported by the Hydrotrope Consortium member companies are:

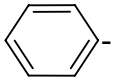
827-21-4	xylene sulfonic acid, sodium salt
28088-63-3	xylenesulfonic acid, calcium salt
30346-73-7	xylenesulfonic acid, potassium salt
16106-44-8	toluenesulfonic acid, potassium salt

Synonyms are listed in Section 1.1 of the SIAR

(3) Substance Formula and Structure:
Diagrams of sodium salts for each of the three hydrotropes (without isomer orientation) are depicted below. Commercial toluene and cumene sulfonates consist of mixtures of 3 isomers (ortho-, meta- and para-). Commercial xylene sulfonic acid consists of mixtures of 6 isomers. An ortho-isomer would have adjacent attachment points to the benzene ring; a para-isomer would have attachments at opposite ends of the benzene ring; and a meta-isomer would have one open carbon between attachments on the benzene ring.


$-CH_3$ $-SO_3Na$ toluenesulfonic acid, sodium salt


$-(CH_3)_2$ $-SO_3Na$ xylenesulfonic acid, sodium salt


$-CH.(CH_3)_2$ $-SO_3Na$ cumenesulfonic acid, sodium salt

(4) Physical Form:
Solid at room temperature; melting point >100°C.

Supplied to formulators as aqueous solutions (30-60% active substance) or solids containing >88 to 100% active substance.

(5) Other Constituents (If Applicable):
Not applicable

II. Summary

(1) Data Collection Efforts:
Information in this assessment was assembled from a number of sources:

1) Member company surveys of the Hydrotropes Consortium (including producers and formulators representing the majority of hydrotrope production in the U.S. and Europe), The Soap and Detergent Association (SDA) (U.S.), and the Cosmetics, Toiletries and Fragrances Association (CTFA)(U.S.) were used to collect data on hydrotrope production volumes, uses, releases, and potential exposures. To protect proprietary information, an independent third party compiled the survey data. The compiled results were confirmed by comparison with a 2002 economic review in the Chemical Economics Handbook by SRI international, and US EPA's summary of 2002 Inventory Update Rule (IUR) information. (Format A)

2) The Australian Government regulator of industry chemicals, the National Industrial Chemicals Notification and Assessment Scheme (NICNAS) conducted a survey on hydrotrope production volumes, product formulations and uses, releases, and potential exposures for Australia. (Format A)

3) Potential hydrotrope exposures are estimated via conservative modelling and summarized in Format C attachments. Potential aquatic exposures resulting from hypothetical U.S. manufacturing facility upper-bound discharges to wastewater are modelled using the E-FAST model from USEPA. The modelled scenario is a general manufacturing release assessment with very high-end release assumptions, not a site specific assessment with actual release data. The model also permits estimation of indirect human exposure from drinking water and consumption of fish downstream of effluent discharges. Similarly, E-FAST is also used to estimate potential upper-bound aquatic exposures and indirect human exposures resulting from consumer use of hydrotrope-containing products (i.e., down-the-drain releases). Finally, direct, upper-bound exposures from consumer uses of products containing hydrotropes are examined using general exposure models for four exposure scenarios: 1) use of diluted liquid detergents (hand-wash of dishes, hand washing of laundry, laundry pre-treatment); 2) use of undiluted hard surface cleaning products; 3) exposure to laundry product residue on clothing (liquid and powder laundry detergents); and 4) exposure to personal care products during and after use (shampoo, hair conditioner, body wash, liquid hand & face soap).

(2) Discussions of Key Uncertainties, Limitations, Data Gaps:
Exposure estimates for aquatic life are based on releases of 100% of total production/importation volume in a geographic region. While there is some uncertainty in the precision of these estimates, the tonnages represent the data from the major manufacturers and are the volumes reported, as required, to regulatory authorities. The models used to predict receiving water concentrations are based upon conservative models that are generally accepted by authorities for screening-level evaluations. The human exposure assessment also uses a conservative (protective) approach to modelling, selecting inputs based on conservative values for each parameter. For example, all

modelled exposures include a default assumption of 100% dermal absorption of hydrotropes. This leads to an overestimate of exposure. A few of the consumer use scenarios are not modelled (e.g., toilet treatments, carpet cleaners), however, formulation information presented for all products and

general knowledge of use patterns/frequency establish these scenarios as being adequately represented by the product use scenarios that are modelled in detail.

(3) Exposure Results:
The following tables show the estimated exposure for the scenarios assessed, and the PNEC or NOAEL hazard values.

Environmental Exposure Scenarios

Exposure Scenario	Concentration (µg/L)	PNEC (µg/L)
Modelled Surface Water Concentrations for Hypothetical U.S. Manufacturing Facility		
Aquatic Exposure – 0.1 tonnes/day		
Mid-size stream with average flow	16.5	2,300
Small stream with low (7Q10) flow	286.9	
Modelled Surface Water Concentrations for Consumer down-the-drain Release		
Aquatic Exposure – 28,684 tonnes/yr (~79 tonnes/day)		
Mid-size stream with average flow	0.048	2,300
Small stream with low (7Q10) flow	0.63	

Consumer Exposure Scenarios

Exposure Scenario	Estimated Exposure (mg/kg bw/day)	NOAEL (mg/kg bw/day)
Indirect Exposure – Manufacturing Effluent Modelling		
Drinking Water Consumption -		
Mid-size stream with average flow	1.1×10^{-4}	763
Small stream with low (7Q10) flow	1.56×10^{-3}	
Fish Consumption -		
Mid-size stream with average flow	4.72×10^{-8}	
Small stream with low (7Q10) flow	6.69×10^{-7}	
Indirect Exposure – Consumer down-the-drain Modelling		
Drinking Water Consumption -		
Small stream with low (7Q10) flow	1.23×10^{-5}	763
Fish Consumption -		
Small stream with low (7Q10) flow	2.63×10^{-8}	
Dermal Modelling		

Face and hand soaps (liquid) Shampoos Hair conditioners Others – including laundry detergents, hand dishwashing liquid detergent, machine dishwashing rinse aid, hard surface cleaners and body washes	0.11 – 0.17 0.03 – 0.14 0.02 – 0.11 0.01 – 0.08	440
Note : range of estimated exposures for dermal modelling represent the range of hydrotrope concentration in product formulations		

III. Production, Import and Use

(1) Estimated Volumes (tonnes/yr):

U.S. - 28,684 (2001 data; consistent with USEPA 2002 IUR)

Europe - 19,348 (2001 data)

Australia - 1,100 (2003 data)

(2) Function/Product Use Categories:

Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients. Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

IV. Activities, Releases and Exposures – Factors that Mitigate or Exacerbate Exposures

Manufacture

(1) Process Description:

Hydrotropes are produced by sulfonation of aromatic hydrocarbon solvents (i.e., cumene, toluene, and xylene). The resulting aromatic sulfonic acid is neutralized utilizing the appropriate base (e.g., sodium hydroxide) to produce the sulfonate or hydrotrope. Liquid product is produced in a closed system. Granular product is produced by spray drying that includes source control and dust collection. Hydrotropes are manufactured for industrial/professional and consumer use and are not used as intermediates/derivatives for further chemical manufacturing processes or uses.
In Australia, the process is partially closed at one site and complete closed at a second site.

(2) General Description of Potential Releases and Exposures:

Hydrotropes are water soluble (>1000 mg/L) and have very low volatility (vp <2.0 x10^{-5} Pa). They are effectively removed in biological wastewater treatment (~94%) and are rapidly and completely biodegraded (>60% in ≤28 days). These characteristics reduce environmental exposure.

Based on EQC Level I modelling (i.e., environmental partitioning estimation as detailed in Mackay et al 1996 and included in Format C), hydrotropes do not partition to any significant degree into soil, sediment, air or biota. The water compartment is the focus for environmental exposure.

For Australia:

Exposures: For facility with partially closed process, unheated, pumped solution is manually packaged into drums. Takes approximately 30 hours and is done 6 times per year.

For U.S.:

Releases: Potential releases to the environment include some stack emission, discharge to wastewater treatment systems and to landfills. Daily release to wastewater treatment is estimated at 0.15% (USEPA default process loss) of annual volume of chemical produced at typical U.S. facility.

Exposures: Estimated receiving water exposures are provided in Format C. Workplace occupational exposures are possible as a result of dermal contact and/or inhalation and ingestion of dust, but are not further quantified.

(3) Discussion of Factors that Decrease or Increase Releases and Exposures:

For Australia:

For facility with partially closed process, there is general and point source ventilation, workers wear goggles, protective clothing, and gloves (acid resistant). For facility with closed process, there is exhaust ventilation; workers wear overalls, eye protection, protective footwear and rubber gloves.

For U.S.:

Environmental releases are regulated as part of overall facility emissions. Mitigation includes using good manufacturing practices, best available technology and engineering controls.

As a result of engineering controls (e.g., exhaust ventilation systems and dust collection) and personal protective equipment (e.g., protective clothing, eyewear and gloves) that would normally be in place at facilities that manufacture liquid and granular materials and/or that formulate products with hydrotropes, the exposure incidental to hydrotropes is decreased. No special engineering controls or additional personal protective equipment are specified for hydrotropes.

MSDS information and product labels for the hydrotropes themselves instruct persons to avoid contact with skin and eyes and to wear eye protection and gloves when handling.

(4) Remarks:

Formulation
(1) Volumes: Essentially all the production volume of hydrotropes is going into product formulation
(2) Process Description: Depending upon the amount of formulated product and level of hydrotrope, hydrotropes can be received in a variety of ways, from totes to truck trailers to rail cars. In Australia, liquid products are formulated by decanting, pump or direct manual addition. For example, hand pumping from 200 L drums into 25 L pails which are then sealed until required for formulation. Packing processes include: gravity filling by weight into packs ranging from 10-1000 L; hydraulic filling of small packs by volume; semi-manual decanting through a hose with tap and dip-leg; semi-automated dosing; and pump through filling lines to bulk storage tanks. No heating was involved at any stage. For granular product, there is a partially closed process where bags containing the pellet form are cut open and added to a tank via a manhole. Addition time is 10 minutes, total mix time is 8 hours, approximately 5 batches per year. This is a heated process (60-65 °C). Samples are collected with a scoop and there are both automated and manual packing processes. In the U.S., for liquid dish or laundry cleaning products, hydrotropes are received in trailers, rail cars or tankers and pumped into heated storage tanks (32-50°C) to prevent salt precipitation. Dish or laundry products can be produced in continuous liquids process (CLP) or batch processes that consist of pipes, mixing tanks, mixers, pumps, heat exchangers, fillers and packaging equipment. The hydrotropes are added to the formulation by controlled flow in-line injection or pumping (batch). The CLP is a completely closed system. The batch system is partially closed.
(3) General Description of Potential Releases and Exposures: Product formulation, the blending of hydrotropes with other ingredients, is not expected to result in releases or workplace or environmental exposures that exceed those for hydrotrope production facilities. For Australia: Formulation processes ranged from open to partially-closed to fully enclosed. The chemical was added to tanks via decanting, pump, or direct manual addition. Batches on average took 2-4 hours, although some were longer (e.g., one full day), and were done daily, to several times a week, to once or twice a year. No atmospheric monitoring is undertaken during this process.

(4) Discussion of Factors that Decrease or Increase Releases and Exposures:

For Australia:

No heating of the product was involved at any of the sites. PPE was worn at all sites.

For U.S.:

Environmental releases are regulated as part of overall facility emissions. Mitigation includes using good manufacturing practices, best available technology and engineering controls.

As a result of engineering controls (e.g., exhaust ventilation systems and dust collection) and personal protective equipment (e.g., protective clothing, eyewear and gloves) that would normally be in place at facilities that manufacture liquid and granular materials and/or that formulate products with hydrotropes, the incidental exposure to hydrotropes is decreased. No special engineering controls or additional personal protective equipment are specified for hydrotropes.

MSDS information and product labels for the hydrotropes themselves instruct persons to avoid contact with skin and eyes and to wear eye protection and gloves when handling.

(5) Remarks:

Commercial/Occupational (or Industrial) Use
(1) Volumes: In Australia, approximately 55 tonnes per year is used as an ingredient in liquid sulphur textile dyes present at 7.5 – 50%, acidic recirculation cleaning present at 10-25%, wetting agent for tanning industry present at 10%, enzymatic recirculation cleaner for dairy and food processing applications at 4%, coolant system conditioner at 6.9%, car wash detergents at 1.3–6.3%, cleaners and degreasers at 0.1–6.3%, vinyl, plastic rubber restorer at 0.2% and floor stripper at 2.7–9 %. In U.S., the fraction of the total 28,684 tonnes per year is not quantified, however, commercial/professional products include hard surface cleaner products where hydrotropes are present at 0.1 to 5.0% .
(2) Process Description: In Australia, information was available on the use textile dyes containing hydrotropes to dye cotton and viscose fibres. Dyes are transferred from 1000 L transport tanks to storage tanks in a closed process. The tanks in which dying takes place are also enclosed. After passing through a dye bath the fabric is subjected to a steam process for the dye to react with the fabric fibres. The fabric then passes through water baths with oxidizing agent to fix the dye to the fabric. Steaming and washing operations and subsequent fabric drying all take place within enclosed systems with exhaust ventilation.
(3) General Description of Potential Releases and Exposures: (a) Releases: Environmental release from down-the-drain discharges following product use. (b) Exposures: Receiving waters may be exposed to hydrotropes following wastewater treatment. Dermal exposure may occur with commercial/professional product use. Exposure from incidental / accidental ingestion, inhalation, and/or eye contact is expected to be less than for dermal contact. In Australia, any waste liquor from the dyeing operation will be highly diluted as a result of large volumes of water which is used for washing off the oxidized dyestuff. No skin contact by workers is expected due to the enclosed or semi-enclosed tank systems in use and precautionary PPE.
(4) Discussion of Factors that Decrease or Increase Releases and Exposures: Hydrotropes are highly water soluble (>1000 mg/L) and have very low volatility (vp $<2.0 \times 10^{-5}$ Pa). They are effectively removed in biological wastewater treatment (~94%) and are rapidly and completely biodegraded (>60% in ≤28 days). These characteristics reduce environmental exposure. Human exposure via inhalation is likely minimal due to low volatility of hydrotropes. Dermal exposure is minimised by use of personal protective equipment. In the Australian dyeing operation, waste liquids are processed via a settling pond and on-site water treatment plant. Operators are equipped with protective gloves, glasses and protective clothing.
(5) Remarks: Human exposures are not modelled separately for commercial/occupational (industrial) uses in this evaluation since the consumer use scenario would represent a more highly exposed individual as a result of frequency of use and the direct application to skin of products containing hydrotropes.

Consumer Use

(1) Function/ Product Use Description:
Hydrotropes are expected to have wide spread and dispersive uses in the following consumer products -

Product Type	Concentration in Products in U.S. (range)	Concentration in Products in Australia (range)
laundry detergents		0.9 - 1.375%
- powders	0.1 – 0.5 %	
- liquids	1 – 10 %	
hard surface cleaners, including dilutable forms	0.1 – 5.0 %	0.1 - 0.9%
machine dishwashing rinse aid	1 – 5%	4.1 - 5.5%
hand dishwashing liquid detergents	1 – 5 %	1.2 - 5.5%
body washes	0.1 – 0.5 %	-
shampoo	1 – 5 %	0.4 - 0.8%
hair conditioner	1 – 5 %	-
face and hand soap (liquid)	10 – 15 %	-
toilet treatments	-	0.2%
solvent hand cleaner	-	0.8%
carpet cleaners	-	1%
optical brightener product	-	3%

Except where noted, the concentration (%) in products shown above is in the formulated product and does not take into account any dilution prior to or during use.

(2) General Description of Direct Exposures to Private (Consumer) Products and of Potential Releases to the Environment Leading to Ecological Exposures and Indirect Human Exposures:
(a) Releases: Environmental release from down-the-drain discharges following product use.
(b) Exposures: Receiving waters may be exposed to hydrotropes following wastewater treatment. Exposure estimates are presented in Format C.
The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, inhalation of, and/or eye contact with product during handling and use. Personal care products are likely to be used daily. Laundry and cleaning products may be used as is, or diluted prior to or during use. Exposure estimates are presented in Format C.

(3) Discussion of Factors that Decrease or Increase Releases and Exposures:
Hydrotropes are highly water soluble (>1000 mg/L) and have very low volatility (vp <2.0 x10^{-5} Pa). They are effectively removed in biological wastewater treatment (~94%) and are rapidly and completely biodegraded (>60% in ≤28 days). Based on physico-chemical properties, the potential for bioaccumulation in aquatic organisms is low. These characteristics reduce environmental exposure.
Human exposure as a result of using laundry/cleaning products is decreased by following use/precaution instructions on product labels. Product labels are written to reflect the entire range of chemical components in any given product. Laundry and cleaning products might include eye and skin irritancy cautionary and first aid information (e.g., to rinse thoroughly if exposed). Low volatility minimizes the potential for inhalation.
Human exposure as a result of using personal care products will be reduced for those that are washed/rinsed off. Exposures may increase by frequent and concurrent use of one or more consumer products.

(4) Remarks :
Direct oral exposures are not modelled in this evaluation since these would only occur via accidental ingestion. None of the uses of hydrotropes are in products intended for human consumption.
Potential oral indirect exposure via drinking water and fish ingestion are included in Format C #1 and #2.
Also not modelled is indirect oral exposure from deposition on dishes washed with products containing hydrotropes. Due to the use of dilute solutions of dishwashing products and the rinsing/draining of dishes following the wash, exposure from this source is considered to be insignificant compared to the direct, dermal exposures that are modelled.
A few products with very low hydrotrope concentrations and/or products that are infrequently used are not modelled (e.g., toilet treatment, carpet cleaners). Potential exposures from these products are considered negligible compared to the products that are modeled.

Format B: Monitoring Evaluations

I. Identification Information

(1) Study Title: none available
(2) Activity Associated with Monitoring Information: Monitoring not considered necessary for exposure assessment of the hydrotropes category. Conservative modelling exposure estimates (see format C) indicate low concern associated with human and environmental exposures. In addition, these chemicals are well removed in wastewater treatment, are rapidly and completely biodegraded, and have low potential for bioaccumulation following environmental release.

II. Monitoring Study Design

(1) Monitoring Study Objective and Scenario Description:

III. Sampling and Analytical Methods

(1) Media Sampled:
(2) Sampling:
(3) Method/ Procedure:

IV. Results and Reliability Description

(1) Results:
(2) Reliability Rating:
(3) Remarks:

Format C: Modelling Evaluation #1
Release and Exposure from US Production Facility

I. Identification Information

(1) Activity Associated with Modelling Information: U.S. manufacturing/production facility effluent discharge – Environmental exposure including both aquatic life and indirect human exposure

II. Modelling Objective

(1) Modelling Study Objective: Screening level estimate (high-end to bounding) of surface water concentration as well as aquatic life, drinking water and fish consumption exposures as a result of manufacturing/production facility effluent discharge.
(2) Description of Modelled Scenario: Accounts for wastewater treatment, in-stream dilution and bioaccumulation potential. Daily process loss/release is estimated at 0.15% (USEPA default process loss) of annual volume of chemical produced. Daily release estimated for a hypothetical "largest" U.S. manufacturing facility and assumes 350 days of operation per year (15 days for annual maintenance). The modelled scenario is a general manufacturing release assessment with very high-end release assumptions (e.g., half the total U.S. production is from this single, hypothetical facility), not a site specific assessment with actual release data. Release from formulation process is not expected to exceed those for production facility.

III. Description of Model and Model Validation

(1) Tool or Model: E-FAST (Exposure & Fate Assessment Screening Tool); Provides screening level estimates of the concentrations of chemicals released to the environment from industrial discharge. Designed to provide high-end to bounding estimates of exposure. Chemical-specific and facility-specific data or defaults can be used. Modelling conducted 2003.
(2) Validation/ Peer Review: Standard model (USEPA 2002) used by USEPA Office of Pollution Prevention and Toxics in screening level assessments
(3) Availability and Documentation: www.epa.gov/oppt/exposure/docs/efast.htm

IV. Inputs, Outputs, and Quality Description

(1) Media Modelled: Surface water, drinking water and edible fish tissue
(2) Inputs:

Pre-treatment release (process losses) per facility = 0.1 tonnes (or 100 kg)/day; estimated as follows:
- 28,684 tonnes/yr = annual production
- 82 tonnes/day = daily production assuming 350 days/year
- 0.123 tonnes/day = daily process loss assuming 0.15% loss
- based on survey conducted by SDA, no single facility produces more than half the total annual production, therefore a conservative assumption is that the maximum daily process loss for a single facility is 0.123 tonnes (or 123 kg)/day or one-half the total daily process loss for the total USA production.

SIC Code is Soaps, Detergents, etc. Manufacture (2841-2844)
Release days = 350
Wastewater treatment removal = 94%
BCF estimate ~3 based on log Kow <1.0 (based on BCFWIN model; USEPA 2003)
PNEC = 2.3 mg/L (lowest EC_{50} for 3 species [fish, daphnia and algae] = 230 mg/L ÷ 100 = 2.3 mg/L) = 2,300 µg/L; where 100 is the recommended assessment factor (Cowan et.al. 1995, OECD 2003, EU 2003)

(3) Model Outputs :
Results following wastewater treatment; where 50% ile represents a large facility on a mid-size stream and 10% ile represents a large facility on a small stream. Two stream flow scenarios (7Q10 = low flow ; mean flow) are modelled.

Aquatic life exposure -
50% ile facility -
Mean stream concentration = 5.9 µg/L
7Q10 stream concentration = 16.5 µg/L
[7Q10 is the lowest 7-day average flow in a year that occurs during 7 consecutive days on average once every 10 years]
10% ile facility -
Mean stream concentration = 83.4 µg/L
7Q10 stream concentration = 286.9 µg/L

Drinking water exposure -
50% ile facility -
Average Daily Dose (ADD) =
1.1×10^{-4} mg/kg bw/day (chronic non-cancer)
10% ile facility -
Average Daily Dose (ADD) =
1.56×10^{-3} mg/kg bw/day (chronic non-cancer)

Fish consumption exposure –
50% ile facility -
Average Daily Dose (ADD) =
4.72×10^{-8} mg/kg bw/day (chronic non-cancer)
10% ile facility -
Average Daily Dose (ADD) =
6.69×10^{-7} mg/kg bw/day (chronic non-cancer)

(4) Reliability Rating:
The reliability rating is 2 (reliable with restrictions). The model has not been validated but is sufficiently conservative and accepted by authorities. The modelling for hydrotropes falls into the applicability domain of the model and appropriate (conservative) inputs were used. Modelling can be useful in first tier approach for exposure assessment. Model outputs reflect E-FAST model assumptions that are designed to provide high-end to bounding estimates of exposure.

(5) Remarks:
The aquatic PNEC = 2300 ug/L (as described in "(2) Inputs"). The high-end to bounding PEC estimates range from 3.9 to 286.9 µg/L and include medium size stream with average flow to small stream with low (7Q10) flow.

The most appropriate NOAEL for an oral exposure scenario is 763 mg a.i./kg bw/day based on a reduction in spleen weight in female rats. The highest estimated average daily doses (ADDs) are 1.56 $x10^{-3}$ mg/kg bw/day (drinking water) and 6.69 $x10^{-7}$ mg/kg bw/day (fish consumption) for the small stream and low (7Q10) flow scenario.

Format C: Modelling Evaluation #2
Release and Exposure from Consumer Use: USA Scenario

I. Identification Information

(1) Activity Associated with Modelling Information: U.S. wastewater treatment facility effluent discharge following consumer use and down-the-drain disposal; environmental exposure including both aquatic life and indirect human exposure

II. Modelling Objective

(1) Modelling Study Objective and Scenario Description: Screening level estimate (high-end to bounding) of surface water concentration (including drinking water and fish consumption exposures) as a result of daily consumer usage of personal care and cleaning products.
(2) Description of Modelled Scenario: Down-the-drain release of total U.S. annual production volume into total volume of U.S. municipal wastewater system. Accounts for wastewater treatment and in-stream dilution. Accounts for bioaccumulation potential

III. Description of Model and Model Validation

(1) Tool or Model: E-FAST (Exposure & Fate Assessment Screening Tool): Provides screening level estimates of the concentrations of chemicals released to the environment from consumer products. Designed to provide high-end to bounding estimates of exposure. Chemical specific data or defaults can be used. Modelling conducted 2003
(2) Validation/ Peer Review: Standard model (USEPA 2002) used by USEPA Office of Pollution Prevention and Toxics in screening level assessments
(3) Availability and Documentation: www.epa.gov/oppt/exposure/docs/efast.htm

IV. Inputs, Outputs, and Quality Description

(1) Media Modelled: Surface water, drinking water and edible fish tissue
(2) Inputs: Release = 28,684 tonnes/yr = annual USA production Wastewater treatment removal = 94% BCF estimate ~3 (based on log Kow <1) (based on BCFWIN model; USEPA 2003) PNEC = 2.3 mg/L (lowest EC_{50} for 3 species [fish, daphnia and algae] is 230 mg/L ÷ 100 = 2.3 mg/L) = 2,300 µg/L; where 100 is the recommended assessment factor (Cowan et.al. 1995, OECD 2003, EU

2003)

(3) Model Outputs:

Aquatic life exposure -

The surface water concentration estimate under median stream flow conditions = 0.048 µg/L. The surface water concentration estimate under low stream flow (7Q10) conditions = 0.63 µg/L.
Indirect human exposure estimates under low stream flow (7Q10) conditions are:

Drinking water exposure –

Average Daily Dose (ADD) =
1.23×10^{-5} mg/kg bw/day (chronic non-cancer)

Fish consumption exposure –

Average Daily Dose (ADD) =
2.63×10^{-8} mg/kg bw/day (chronic non-cancer)

(4) Reliability Rating:

The reliability rating is 2 (reliable with restrictions). The model has not been validated but is sufficiently conservative and accepted by authorities. The modelling for hydrotropes falls into the applicability domain of the model and appropriate (conservative) inputs were used. Modelling can be useful in first tier approach for exposure assessment. Model outputs reflect E-FAST model assumptions that are designed to provide high-end to bounding estimates of exposure.

(5) Remarks:

The aquatic PNEC = 2300 ug/L (as described in "(2) Inputs"). The high-end to bounding PEC estimates range from 0.048 to 0.63 µg/L and include medium size stream with average flow to small stream with low (7Q10) flow.

The most appropriate NOAEL for an oral exposure scenario is 763 mg a.i./kg bw/day based on a reduction in spleen weight in female rats. The highest estimated average daily doses (ADDs) are 1.23×10^{-5} mg/kg bw/day (drinking water) and 2.63×10^{-8} mg/kg bw/day (fish consumption) for the small stream and low (7Q10) flow scenario.

Format C: Modelling Evaluation #3
Release and Exposure from Consumer Use: Australia Scenario

I. Identification Information

(1) Activity Associated with Modelling Information: Australia wastewater treatment facility effluent discharge following consumer use and down-the-drain disposal; environmental exposure including both rivers and ocean waters.

II. Modelling Objective

(1) Modelling Study Objective and Scenario Description: Screening level estimate (high-end) of surface water concentration as a result of daily consumer usage of personal care and cleaning products.
(2) Description of Modelled Scenario: Down-the-drain release of total Australian annual manufacturing and import volume into rivers and oceans. Accounts for wastewater treatment and dilution as follows. Dilution in the event of release to rivers is assumed to be negligible. Effluent will constitute the majority, if not all, of river flow in drier months. In the immediate area of ocean release, a dilution of 10:1 is assumed

III. Description of Model and Model Validation

(1) Tool or Model: Simple calculation based on total dispersed use and removal estimate from wastewater treatment. Predicted removal from the sewage treatment plant (STP) using the SIMPLETREAT model (input parameters as follows: LogH<<-4 Pa m^3/mol; Log Kow range of -2.7 to -1.5; readily biodegradable) is 87% by degradation with 13% remaining in the water discharge. Measured data (modified Semi-Continuous Activated Sludge [SCAS] test) indicates removal of 94%.
(2) Validation/ Peer Review: Standard approach in screening level assessments
(3) Availability and Documentation: SIMPLETREAT is published and can be viewed at www.epa.gov/oppt/exposure/docs. The SCAS result is reported in the accompanying dossier for calcium xylene sulfonate (28088-63-3) and in reference Ruetgers-Nease Chemical, Inc., 1994.

IV. Inputs, Outputs, and Quality Description

(1) Media Modelled: River and ocean waters
(2) Inputs: Release = 1100 tonnes/yr = annual Australian manufacture + import; Wastewater treatment removal = 90%; Wide dispersive release over 365 days of the year
(3) Model Outputs: 83µg/L in rivers and 8.3µg/L in ocean water.
(4) Reliability Rating: The reliability rating is 2 (reliable with restrictions). The model has not been validated but is sufficiently conservative and generally accepted by authorities.

Format C: Modelling Evaluation #4
Dermal Exposures from Consumer Uses of Products

I. Identification Information

(1) Activity Associated with Modelling Information:
Human dermal exposures from use of laundry/cleaning and personal care products

II. Modelling Objective

(1) Modelling Study Objective:
The objective of the dermal exposure model for consumer product uses is to estimate "screening" levels of human exposure (in daily dose, i.e. mg/kg bw/day) and compare to the most sensitive toxic endpoint (e.g. lowest NOEL/NOAEL) in order to assess exposure and risk potential. Exposure and risk estimations could then be subjected to further refinement as needed. Because of the conservative nature of the screening level assessment, when product uses are determined to be of low concern, no further evaluation would be conducted.

(2) Description of Modelled Scenarios:
Dermal exposures to hydrotropes that are modelled include:

Exposure during the activity/use of products[1] --
Laundry detergent: hand washing clothes
Laundry detergent: pre-treatment
Dishwashing liquid detergents: hand washing dishes
Hard surface cleaners (diluted and undiluted)
[1]Exposure during the activity/use of personal care products are not modelled because these exposures (lasting just minutes) are very small in comparison to exposure to residuals that last until the next use (e.g., for a day).

Exposure from residuals on clothing –
Laundry detergents on clothing following washing

Exposure from residuals after using products --

Shampoos	Face and hand soap (liquid)
Hair conditioners	Body washes

The exposure scenarios encompass conservative, screening-level assumptions including: the high-end frequency of product use, the high-end amount of product per use, the high-end percent of product retained on skin or clothes following use, and 100% dermal absorption. SDA member companies provided formulation information and the entire range of hydrotropes in specified product types are used in this assessment.

Direct oral exposures are not modelled in this evaluation since these would only occur via accidental ingestion. None of the uses of hydrotropes are in products intended for human consumption. Incidental oral exposure via drinking water and fish ingestion are included in Format C#1 and C#2.

Inhalation exposures are not modelled for hydrotropes. Trigger-spray hard surface cleaners have the potential to aerosolize product, however, the low volatility of hydrotropes and the relatively infrequent use of these products (in comparison to products involving dermal contact) was the basis for not including an inhalation modelling scenario.

III. Description of Model and Model Validation

(1) Tool or Model:

The modelling presented here uses simple, first principle equations, which, when combined with conservative (protective) input values err on the side of being protective.

General Exposure Model

Potential Chemical Exposure (PE) =
Exposure to Product (EXP) x Chemical Concentration in Product Formulation (PF)

Dermal Exposure

1. **Exposure during the activity/use of diluted and undiluted laundry and dishwashing products, and diluted and undiluted hard surface cleaning products**

$$\frac{[FQ \times CA \times PC \times FT \times CF \times TF \times DA]}{BW} \times PF$$

2. **Exposure to laundry product residual on clothing**

$$\frac{[A \times PR \times PT \times DA \times CF]}{BW} \times PF$$

["FQ" (frequency of use) is 1 wash load/day for clothing]

3. **Exposure to residual after using personal care products**

$$\frac{[FQ \times A \times PR \times DA \times CF]}{BW} \times PF$$

Where:

FQ: frequency of use (use/day)
CA: body surface contact area (cm^2)
PC: product concentration (g/cm^3)
FT: film thickness on skin (cm)
CF: conversion factor (1000 mg/g)
TF: time scaling factor (unitless)
DA: dermal absorption (%)
BW: female body weight (kg)
A: amount per use (g/day or g/wash)
PF: Hydrotrope concentration in product formulation (%)
PR: percent retained on clothing or on skin (%)
PT: percent transferred from clothing to skin (%)

(2) Validation/ Peer Review:
These exposure calculations use first principle equations and are mathematically consistent with EPA Exposure Guidelines (1992) with regard to modelling dermal doses.

(3) Availability and Documentation:
USEPA 1992. Guidelines for Exposure Assessment. Washington, DC. Office of Research and Development, Office of Health and Environmental Assessment. EPA/600/Z-92-001.

IV. Inputs, Outputs, and Quality Description

(1) Media Modelled:
The exposure media are the hydrotrope-containing products used by consumers. The Hydrotrope Consortium fielded a survey among producers and formulators to provide the range of hydrotrope contained in each of the product forms. For each product category containing hydrotropes, the minimum and maximum of the range was utilized as inputs for the dermal exposure models. The product formulations reported by Australia (also shown in Format A) are generally comparable; therefore, the human exposure estimates can be considered representative of uses in both countries.

(2) Inputs:

1. Exposure during the activity/use of diluted and undiluted laundry and dishwashing products, and diluted and undiluted hard surface cleaning products

$$\frac{[FQ \times CA \times PC \times FT \times CF \times TF \times DA]}{BW} \times PF$$

	Laundry Pre-treatment	Laundry Hand-wash	Hand Wash Dishes	Hard Surface Cleaners
FQ (use/day)	1 [a]	1 (liq.and powd.) [a]	3 [a]	1 [d]
CA (cm^2)	360 [b]	1680 [f]	1680 [f]	360 [b]
PC (g/cm^3)	0.6 [a]	0.01 [a]	0.0015 [a]	0.2 [a]
FT (cm)	0.0024 [c]	0.0024 [c]	0.0024 [c]	0.0024 [c]
CF (1000mg/g)	1000	1000	1000	1000
TF (unitless)	0.007 [d]	0.007 [d]	0.03 [d]	0.014 [a]
DA (%) [h]	100%	100%	100%	100%
Female BW (kg)	60 [e]	60 [e]	60 [e]	60 [e]
PF (%)[g]	1-10% (liquid) 0.1-0.5% (powder)	1-10% (liquid) 0.1-0.5% (powder)	1-5%	0.1-5%

References:
a: SDA Habit and Practice Survey
b: Palms surface area (USEPA Exposure Factors Handbook)
c: USEPA 1985 (Methods of assessing exposure to chemical substances)
d: HERA project 2002
e: female body weight (USEPA Exposure Factors Handbook)
f: hands and forearms (USEPA Exposure Factors Handbook)
g: Hydrotrope Survey, Min-Max values (see table in section IV. Consumer Use (1))
h: default assumption

2. Exposure to laundry product residual on clothing

$$\frac{[A \times PR \times PT \times DA \times CF]}{BW} \times PF$$

	Liquid Laundry detergent	Powder Laundry detergent
A (g/wash)	121[a]	121[a]
PR (%)	1%[a]	1%[a]
PT (%)	1%[a]	1%[a]
DA(%)	100%[b]	100%[b]
CF (mg/g)	1000	1000
BW (kg)	60 [c]	60 [c]
PF (%)	1-10%[d]	0.1-0.5%[d]

References:
a: SDA Habit and Practice Survey
b: Default assumption
c: female body weight (USEPA Exposure Factors Handbook)
d: Hydrotrope Survey, Min-Max values (see table in section IV. Consumer Use (1))

3. Exposure to residual after using personal care products

$$\frac{[FQ \times A \times PR \times CF \times DA]}{BW} \times PF$$

	Shampoo	Hair Conditioner	Body Wash	Hand & Face Soap (liquid)
FQ	1[a]	1 [a]	1[a]	8[a]
A	16.4[a]	12.7[a]	12 [a]	1.7[a]
PR	1% [b]	1% [b]	0.5% [a]	0.5% [a]
CF	1000	1000	1000	1000
DA[e]	100%	100%	100%	100%
BW	60 [c]	60 [c]	60 [c]	60 [c]
PF[d]	1-5%	1-5%	0.1-0.5%	10-15%

References:
a: SDA Habit and Practice Survey
b: CTFA 2003 data; Min-Max values
c: female body weight (EPA Exposure Factors Handbook)
d: Hydrotropes Survey, Min-Max values (see table in section IV. Consumer Use (1))
e: Default assumption

(3) Model Outputs:

Product Category	Dermal – potential exposure (mg/kg bw/day) [a]
Face and hand soaps (liquid)	0.11 – 0.17
Shampoos	0.03 – 0.14
Hair conditioners	0.02 – 0.11
Others [b]	0.01– 0.08

Footnotes:
a: range based on Min. and Max. "PF" values (i.e., hydrotrope concentration in product formulation)
b: includes laundry detergent (powders and liquids), machine dishwashing rinse aid, hand dishwashing liquid detergent, hard surface cleaners and liquid body washes

(4) Reliability Rating:

The reliability rating is 1 (reliable without restrictions). The model used first principal equations, which are sufficiently conservative, have undergone peer review and are generally accepted by authorities. The modelling for hydrotropes in consumer products falls into the applicability domain of the model and appropriate (conservative) inputs were used. The model used is applicable for screening-level assessment. The selected model inputs reflect best available information and conservative estimates where applicable (i.e., high-end frequency of product use, high-end amount of product per use, high-end percent of product retained, and 100% dermal absorption).

(5) Remarks:

Indirect oral exposure from deposition on dishes was not modelled. Due to the use of dilute solutions of dishwashing products and the rinsing/draining of dishes following the wash, exposure from this source is insignificant compared to the direct, dermal exposures that are modelled.

A few products with very low hydrotrope concentrations and/or products that are infrequently used are not modelled (e.g., toilet treatments, carpet cleaners). Potential exposures from these products are considered negligible compared to the products that are modelled.

In the particular case of hydrotropes, use of all the noted product categories by a single consumer is plausible. That is, an individual could be using laundry cleaning products, machine and/or hand dishwashing detergents, hard surface cleaners, liquid body wash, face and hand soap, shampoos and hair conditioners. A conservative estimate of aggregate daily exposure could therefore be achieved by a simple addition of the daily exposure estimates for each of the product categories. Exposure estimates for drinking water and fish consumption (Format C, Model Evaluation #1 (production facility) and #2 (consumer use); section IV (3) in each) could be added to the total as well.

Appendix 1: References

Cowan, CE, DJ Versteeg, RL Larson and P Kloepper-Sams. 1995. Integrated approach for environmental assessment of new and existing chemicals. Regulatory Toxicol. Pharmacol. 21:3-31

European Union (EU) 2003. Technical Guidance Document on Risk Assessment in Support of Commission Directive 93/67/EEC on Risk Assessment for new notified substances. 337 pp.

HERA. 2002. Guidance Document Methodology. April 2002. http://www.heraproject.com/RiskAssessment.cfm

Hydrotrope Category robust study summaries include physico-chemical, treatment plant removal and aquatic toxicity data

Hydrotropes Survey. 2002. Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

Mackay, D, A DiGuardo, S Peterson and C Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environ. Toxicol.Chem. (15)9: 1627-1637.

OECD. 2003. Manual for Investigation of HPV Chemicals. http://www.oecd.org/document/7/0,2340,en_2649_34379_1947463_1_1_1_1,00.html

SDA Habit and Practice Survey. 2002. Survey conducted by the Soap and Detergent Association and its member companies.

USEPA. 1985. Methods of assessing exposure to chemical substances. Vol. 7, Versar. EPA 560/5-85-007.

USEPA. 1987. Exposure Factors Handbook. August 1987.

USEPA 1992. Guidelines for Exposure Assessment. Washington, DC. Office of Research and Development, Office of Health and Environmental Assessment. EPA/600/Z-92-001.

USEPA 2002. E-FAST model. Office of Pollution Prevention and Toxics. Washington, DC. http://www.epa.gov/oppt/exposure/docs/efast.htm

USEPA 2003. BCFWIN model in EPI Suite. http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Appendix 2: Data Search Strategy

Consortium member companies contributed in-house studies of physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity for the chemicals in the category. To supplement the industry data, literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases. These databases include:

- Registry of Toxic Effects of Chemical Substances (RTECS)
- Hazardous Substances Database (HSDB)
- Aquatic Toxicity Information Retrieval (AQUIRE)
- Toxic Substances Control Act Test Submissions (TSCATS)
- Integrated Risk Information System (IRIS)
- The Environmental Teratology Information Center (ETIC)
- The Developmental and Reproductive Toxicology Database (DART)
- The Catalog of Teratogenic Agents (CTA)
- ENVIROFATE, DATALOG, AQUIRE, PHYOTOX and TERRATOX
- Chemical Carcinogenesis Research Information (CCRIS)
- The Environmental Mutagen Information Center (EMIC)
- GENETOX
- Sax's Dangerous Properties of Industrial Materials
- Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles
- International Uniform Chemical Information Database (IUCLID)
- Environmental Chemical Data Information Network (ECDIN)
- TOXLINE
- www.chemfinder.com
- standard scientific data compendia such as Verschueren (1996), CRC Handbook of Chemistry and Physics and The Merck Index.

CAS Registry Numbers were used to match records available in each database. In addition, the search of the Merck Index, CRC Handbook of Chemistry and Physics and Verschueren included the names of isomers, that is, ortho-, meta- and para- toluene, xylene and cumene sulfonic acids. No records were found for the isomers, however, data reported for the CAS materials would apply to the isomers as well given the CAS materials are mixtures of isomers. All reports identified were subject to a reliability check for determining adequacy in developing the Robust Summaries.

SIDS DOSSIER

CAS NOs. 1300-72-7 (827-21-4)

Xylene sulfonic acid, sodium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

12068-03-0
16106-44-8
26447-10-9
28088-63-3
28348-53-0 (32073-22-6)
30346-73-7
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **1300-72-7**

(also 827-21-4)

B. Name *(IUPAC name* **sodium xylenesulphonate**

(sodium m-xylene-4-sulphonate)

C. Name *(OECD name* **xylene sulfonic acid, sodium salt**

(same)

D. CAS Descriptor **Benzenesulfonic acid, dimethyl-, sodium salt**

(Benzenesulfonic acid, 2,4-dimethyl-, sodium salt)

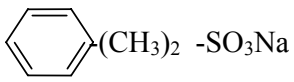
E. EINECS-Number **215-090-9**

(212-567-3)

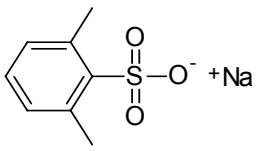
F. Molecular Formula **C8 H9 O3 S1 Na1**

G. Structural Formula

Commercial xylene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the ortho, ortho isomer as a representative structure. A para-isomer would have attachments at opposite ends of the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.



.



H. Substance Group **Hydrotropes category**

I. Substance Remark **The same substance is identified by two CAS numbers**

J. Molecular Weight **208 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country: Australia

B. Lead Organization:

Name of Lead Organization:
National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
Tel: +61 2 8577 8880

C. Name of responder

Name: Kathleen Stanton, Consortium Manager
Address:
The Soap and Detergent Association
1500 K Street, N.W., Suite 300
Washington, D.C. 20005
USA
Tel: (202) 662-2513
Fax: (202) 347-4110

Consortium Participants:
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Name: Konrad Gamon/Roger Johnson
Address:
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Name: John S. Winton
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Name: Hans Certa
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Name: Lela Jovanovich
Address:
Stepan Company
22 West Frontage Road
Northfield, IL 60093
USA

Name: Lionel Godefroy
Address:
Stepan Europe
Chemin Jongkind
38340 Voreppe
France

1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six "sponsored" substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ];
petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate or

1.2 SYNONYMS

xylenesulfonic acid, sodium salt
xylenesulfonate, sodium salt
sodium xylene sulfonate
benzenesulfonic acid (1-dimethyl) sodium salt
dimethylbenzenesulfonate, sodium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%

Carpet Cleaners	-	-	1%
Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: [Na]OS(=O)(=O)c1ccc(cc1C)C MOL FOR: C8 H9 O3 S1 Na1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	EPI-001
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	208.21	
Water Solubility (mg/l):	1e+006	n/a
Octanol Water Partition Coefficient (Log Kow):	-1.86	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	544.57	n/a
Melting Point (°C):	233.42	n/a
Vapor Pressure(mmHg):	1.52E-09	n/a
Henry's Law Constant (atm/(mole/m^3)):	3.123E-018	n/a
Atmospheric Oxidation Half-Life (hours):	41	n/a
Soil Adsorption Coefficient (Log Koc):	1.500	

Remarks: n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference: Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Other References: n/a

Other

Sponsor: n/a

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 2.0.1_1300-72-7_163

Last Revised: 11-4-2005

Remarks: n/a

2.1 MELTING POINT

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: > 93%

Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1997

Report/Study Number: MSDS No. 1-10104

Method/Guideline Followed: not indicated

Analytical Monitoring: n/a

Remarks: n/a

Results

Value:

Operator	Lower (°C)	Upper (°C)
>	300	n/a

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature

Reference

Source Reference: 42 Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® SX / MSDS No. 1-10104. 1997a

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 2.1_1300-72-7_100
Last Revised: 6-19-2004
Remarks: n/a

Test Substance

CAS Number: 827-21-4
Identity: Xylene sulfonic acid, sodium salt
Purity: 99.9%
Remarks: Manufacture: Nacalai Tesque, Inc; Lot No. KCG5267

Method

GLP: no
Report/Study Year: 1996
Report/Study Number: n/a
Method/Guideline Followed: Other: ISO 1218-1975 (E): Plastics – Polyamides – Determination of "melting point"
Analytical Monitoring: n/a
Remarks: n/a

Results

Value: > 300 ˚C. No clear melting point was observed up to 300 degree C
Remarks: n = 2

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; Full study report is available and is well documented.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 62. Chemicals Evaluation and Research Institute (CERI). 1996. Measurement of Melting Point of 2.4-dimethyltoluene sulfonic acid, sodium salt. Unpublished data.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.1_827-21-4_100
Last Revised: 11-04-2005
Remarks: n/a

2.2 BOILING POINT

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: not indicated
Remarks: 30-40% aqueous solution

Method

GLP: n/a
Report/Study Year: 1993
Report/Study Number: SDAHT06
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Pressure:

Value	Unit
1000	hPa

Remarks: n/a

Results

Value: 100 ˚C
Remarks: Result reflects boiling point of aqueous solution and therefore of water. The chemical substance is an ionic solid. Hydrotrope products are produced as either aqueous solutions or as granular solids.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 3 Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.2_1300-72-7_114
Last Revised: 11-04-2005
Remarks: n/a

2.3 DENSITY

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: n/a
Remarks: pellets

Method

GLP: n/a
Report/Study Year: 1993
Report/Study Number: SDAHT06
Method/Guideline Followed: n/a
Test Type: n/a
Temperature (°C): 20
Remarks: Bulk density

Results

Value: 0.45 – 0.55 g/cm^3
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 3. Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.3_1300-72-7_115
Last Revised: 11-04-2005
Remarks: n/a

2.4 VAPOUR PRESSURE

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: 93%
Remarks: White powder

Method

GLP: yes

Report/Study Year: 2005
Report/Study Number: 2098/001
Method/Guideline Followed: Commission Directive 92/69/EEC Method A4
Temperature (°C): 240 – 250 °C
Remarks: n/a

Results

Value: < 2.0 x 10^{-5} Pa at 25°C
Decomposition: not indicated
Remarks: Value at 25°C determined by extrapolation. Measured points were below detection levels and too variable to draw a line of best fit. Instead, a regression slope of -1500 was used (derived from the shallowest slope obtained using the vapour pressure balance method) thus giving a worst case scenario for vapour pressure.

Data Quality

Reliability (Klimisch): 1
Remarks: Reliable without restriction.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 57. SafePharm Laboratories. 2005. Xylene sulfonic acid, sodium salt (93%): Determination of vapour pressure. SPL project number 2098/001.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.4_1300-72-7_116
Last Revised: 11-04-2005
Remarks: n/a

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: n/a
Remarks: pellets

Method

GLP: n/a
Report/Study Year: 1993
Report/Study Number: SDAHT06
Method/Guideline Followed: n/a

Temperature (°C): not indicated
Remarks: n/a

Results

Value: non-volatile
Decomposition: not indicated
Remarks:

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 3. Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.4_1300-72-7_116
Last Revised:	11-04-2005
Remarks:	n/a

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW}

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. log_{10} K_{ow} was measured for CAS number 28088-63-3.

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	n/a

Method

GLP:	not indicated
Report/Study Year:	1993
Report/Study Number:	SDAHT06
Method/Guideline Followed:	not indicated
Analytical Monitoring:	n/a
Solubility Media:	water

pH:

Operator	Lower	Upper
=	8	10

pH Concentration:

Value	Unit	Temp. (°C)
=	8.5	20

Remarks: n/a

Results

Value: 400 g/l at 20 ˚C

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 3. Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 2.6.1_1300-72-7_117

Last Revised: 6-19-2004

Remarks: n/a

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: > 93%

Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1997

Report/Study Number: MSDS No. 1-10104

Method/Guideline Followed: not indicated

Remarks: n/a

Results

Description: Soluble in water

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 42. Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® SX / MSDS No. 1-10104. 1997a

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.6.1_1300-72-7_101
Last Revised:	11-04-2005
Remarks:	n/a

3.0.1 EQC MODEL

Fugacity modelling has been conducted on CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: [Na]OS(=O)(=O)c1ccc(cc1C)C MOL FOR: C8 H9 O3 S1 Na1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 1300727
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	3.11 E-12 cm3/molecule-sec
Half Life	41 hrs
Remarks:	n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File	AOPWOO1 1300727

Name:
Last Revised: 05-09-06
Remarks: n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3. TRANSPORT AND DISTRIBUTION

Refer section 3.0.1 EQC Model.

3.4 BIODEGRADATION

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: 36.34% a.i.
Remarks: Substance tested are aqueous solutions; % purity equates to chemical content

Method

GLP: no
Report/Study Year: 1993
Report/Study Number: 16BF53
Test Type: aerobic
Method/Guideline Followed: OECD 301B. Modified Sturm
Inoculum: Activated sludge
Inoculum Acclimated: no
Control Substance: analine

Test Substance Initial Concentration:

Value	Unit	Expressed as
10	mg/L	OC (organic carbon)
20	mg/L	OC

Control Substance Initial Concentration:

Value	Unit	Expressed as
20	mg/L	OC

Remarks:

- Temperature: 22 ± 2 °C.
- Analysis: CO_2 produced was trapped as $BaCO_3$. Analysis of residual $Ba(OH)_2$ with HCl solution (0.05 N)

- Analysis on day 4, 8, 15 and 28.

Results

Result:

day	4	8	15	28
10 mg Carbon/L	0.85	45.8	74.0	88.3
20 mg C/L	0.40	4.45	68.5	86.0
Reference	19.0	64.4	80.2	89.5

expressed as %$THCO_2$
The substance is readily biodegraded (10-day window is met; >60% degraded); 87% degraded in 28 days.

Remarks: .

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Study was not GLP.

Reference

Source Reference: 46. Stepan Company, Northfield, Illinois, USA. Biotic Degradation (Modified Sturm test) Evaluation, in an aqueous medium, of the "ultimate" biodegradability of substances: 1736-1A, 1736-1B, 1736-1C, 1736-1D, 1736-1E / 16 BF 53. 1993

Other

Sponsor: Stepan Company

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: INERIS, Verneuil-en-Halatte, France

Print File Name: 3.5_1300-72-7_87

Last Revised: 11-04-2005

Remarks: Test substance was used as sole carbon source.

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 40%

Remarks: Substance tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes

Report/Study Year: 1992

Report/Study Number: 40428

Test Type: aerobic

Method/Guideline Followed: OECD 301B. Modified Sturm.

Inoculum: Activated sludge

Inoculum Acclimated: yes

Acclimated to what Concentration: 20 mg C/L

Acclimated for what Duration: 19 days

Control Substance: Sodium acetate

Test Substance Initial Concentration:

Value	Unit	Expressed as
10	mg/L	OrganicCarbon (OC)
20	mg/L	OC

Control Substance Initial Concentration:

Value	Unit	Expressed as
20	mg/L	OC

Remarks:

- Pre-acclimation phase: 9 days thereafter SCAS test.
- Acclimation of sludge for SCAS test: adapted to 20 mg C/L for 19-days at 22 ± 3 °C.
- Temperature: 22 ± 3 °C.
- Analysis: CO_2 produced was trapped in the 0.2 N KOH solutions in the gas-washing bottles.
- Analysis on day 2, 4, 6, 8, 10, 15, 20, 25 and 28.

Results

Result:

day	2	4	6	8	10	15	20	25	28
10 mg Carbon/L	3.32	3.32	21.04	51.22	59.82	74.23	79.82	80.29	83.88
20 mg C/L	2.53	2.53	26.22	46.14	52.94	63.51	66.83	67.39	69.30
Reference	17.85	29.00	80.81	83.15	85.30	92.62	93.21	93.21	93.21

Reported as %$THCO_2$
The substance is biodegradable, more than 60% after 15 days

Remarks: 74% degraded in 15 days; 84% in 28 days at 10 mg C/L

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 33. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Evaluation for biodegradability in the Modified Sturm Test of Sodium xylenesulfonate [1300-72-7]. 1992c

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory:	ABC Laboratories Inc., Colombia, Missouri, USA
Print File Name:	3.5_1300-72-7_88
Last Revised:	11-04-2005
Remarks:	Pre-acclimation: The pH was adjusted with dilute HCl to maintain a pH that ranged from 6.5 to 8.0. Biodegradability follows from acclimated as well as unacclimated units.

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	1965
Report/Study Number:	SDAHT04
Test Type:	aerobic
Method/Guideline Followed:	not indicated
Inoculum:	Two systems, one with natural river microbial flora, the other with raw municipal sewerage.
Inoculum Acclimated:	no
Control Substance:	none

Test Substance Initial Concentration:

Value	Unit	Expressed as
10	mg/L	test substance

Remarks:

- The second system consisted of distilled water containing 5 ppm of yeast extract and was inoculated with 5 mL/liter of raw municipal sewage.
- Analysis: by photospectrometric method (UV). Measured test substance against a blank.
- Temperature: 25 °C.

Results

Result: Degradation of Xylene sulfonate after 8-days: 100%

	1 day	2 days	3 days	4 days	5 days	6 days	7 days	8 days
Xylene sulfonate	0%	9%	18%	47%	69%	72%	75%	100%

Remarks:

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Not a generally accepted method

Reference

Source Reference: 6. Continental Oil Company. Detergent Hydrotropes/Foam Stabilizers, from Soap and Chemical Specialties. 1965

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 3.5_1300-72-7_91

Last Revised: 6-29-2004

Remarks: The two biological test systems were found to produce essentially identical results.

Test Substance

CAS Number: 827-21-4

Identity: Xylene sulfonic acid, sodium salt

Purity: 99.9%

Remarks: Manufacture: Nacalai Tesque, Inc; Lot No. KCG5267

Method

GLP: yes

Report/Study Year: 1996

Report/Study Number: 21326

Test Type: aerobic

Method/Guideline Followed: OECD Guideline 301C “Ready biodegradability: Modified MITI Test (I)”

Inoculum: Activate sludge

Inoculum Acclimated: no

Control substance: Aniline

Test Substance Initial Concentration:

Value	Unit	Expressed as
100	mg/L	test substance

Remarks: 30 mg of the test substance (n=3) or aniline (n=1) and 9 mg of activated sludge (as MLSS) were added into 300 ml of test medium. Before adding the inoculum, pH values were adjusted to 7 +/- 0.1 by HCl. The test and control vessels were cultivated for 28 days at 25 degree C. Biodegradability

continuously measured by a BOD meter. At the end of the test, residual amount of the test substance was determined by TOC and HPLC analysis.

Results

Under test conditions, no biodegradation observed.

Degradation kinetics:

Result:

	7 day	14 days	21 days	28 days
xylene sulfonate	0%	0%	0%	0%
Aniline	49%	72%		

Remarks: pH in the test solution at the end of the test were 7.3. 7.5, 7.9

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Full study report is available and is well documented.

Reference

Source Reference: 63. Chemicals Evaluation and Research Institute (CERI). 1996. Final Report of Biodegradability Study of 2,4-dimethyltoluene sulfonic acid, sodium salt. Report Number 21326. Unpublished data.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 3.5_827-21-4_90

Last Revised: 11-04-2005

Remarks: While a valid test, these results (i.e., “non-biodegradable”) are inconsistent with the results (i.e., “biodegradable”) obtained from the other biodegradation test with toluene sulfonic acid, sodium salt as well from 9 biodegradation tests with the other chemical substances that make up the hydrotropes category.

3.6 BIOACCUMULATION

Test Substance

CAS Number: 827-21-4

Identity: Xylene sulfonic acid, sodium salt

Purity: 99.9%

Remarks: Manufacture: Nacalai Tesque, Inc;
Lot No. KCG5267

Method

GLP:	yes
Report/Study Year:	1996
Report/Study Number:	51326
Method/Guideline Followed:	OECD Guideline 305C: Bioaccumulation, Test for the degree of bioconcentration in Fish.
Species:	*Cyprinus sp.* (freshwater fish)
Exposure Period:	42 days at 25 degree C
Remarks:	A number of fish were exposed to concentrations at 0.5 and 0.05 mg/L under flow through system. Test concentrations in water and fish were determined by HPLC analysis.

Results

BCF <2.3

Remarks: All measured BCF values were lower than detection limit of HPLC analysis.

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions. Full study report is available and is well documented.
Flag	Critical study for SIDS endpoint

Reference

Source Reference: 64. Chemicals Evaluation and Research Institute (CERI). 1996. Final Report of Bioaccumulation Study of 2,4-dimethyltoluene sulfonic acid, sodium salt. Report Number 51326. Unpublished data.

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	3.7.1_827-21-4_104
Last Revised:	11-04-2005
Remarks:	n/a

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	40.77%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	no
Report/Study Year:	1993
Report/Study Number:	13039.0393.6103.103
Method/Guideline Followed:	EPA-TSCA 797.1400
Test Type:	acute, static
Analytical Monitoring:	no
Species:	Rainbow trout (*Onchorhynchus mykiss*) , length 32-45 mm.

Exposure Period:

Value	Unit
96	hour(s)

Remarks: Number of fish: 10/test vessel, 2 test vessels/treatment.
Concentrations: Nominal: 130, 220, 360, 600 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Test conditions: Static without aeration; at 12±1 °C in 19 L glass vessels containing 15 L of medium of hardness 36 mg/L (as $CaCO_3$) and pH 7.5; 16 hours light; unfed.
Physical measurements: at 0, 24, 48, 72 and 96 hours: overall ranges for pH 7.0-7.4; O_2 78-92%; temperature 11-13 °C.
Observations: Mortality/symptoms at 0, 24, 48, 72 and 96 hours.

Results

Unit: mg/L

Results:

		Nominal concentration (mg/L)					
Parameter	Time [hour]	0	130	220	360	600	1000
Mortality [%]	96	None					
Symptoms	0-96	No treatment related effects					

96-hr LC50 > 1000 mg/L (equivalent to >408 mg/L active ingredient taking into account the 40.7% purity of the sample)

Minor remark Fish were smaller than the 40-60mm recommended by OECD 203. Since

smaller fish may be more sensitive, the outcome of the study was not affected.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Non GLP, no analyses

Reference

Source Reference: 48 Stepan Company, Northfield, Illinois, USA; Stepanate SXS – Acute Toxicity to Rainbow Trout (*Oncorhynchus mykiss*) under static conditions / 13039.0393.6103.103, 1993c

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Springborn Laboratories Inc., Wareham, Massachusetts, USA

Print File Name: 4.1_1300-72-7_1

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 40%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes

Report/Study Year: 1992

Report/Study Number: 40422

Method/Guideline Followed: EPA-TSCA 797.1400.

Test Type: acute, static

Analytical Monitoring: no

Species: *Pimephales promelas*, mean length 25 ± 4 mm.

Exposure Period:

Value	Unit
96	hour(s)

Remarks: Statistical method: Binominal, moving average and probit analysis.
Number of fish: 10/test vessel, 2 test vessels/treatment.
Concentrations: Nominal: 100, 180, 320, 560 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for

sample purity.
Test conditions: Static without aeration; at 22 ± 1 °C in 19 L glass vessels containing 15 L of medium of hardness 144 mg/l (as $CaCO_3$) and pH 7.7; 16 hours light; unfed.
Physical measurements: at 0, 48 and 96 hours: overall ranges for pH 7.9-8.3; O_2 84-92%; temperature 22-23 °C.
Observations: Mortality/symptoms at 24, 48, 72 and 96 hours.

Results

Unit: mg/L

Results:

		Nominal concentration (mg/L)					
Parameter	Time [hour]	0	100	180	320	560	1000
Mortality [%]	96	None					
Symptoms	0-96	No treatment related effects					

96-hr LC50 > 1000 mg/L (equivalent to >400 mg/L active ingredient taking into account the 40% purity of the sample).

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. No analyses

Flag Critical study for SIDS endpoint

Reference

Source Reference: 20 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA, Static acute toxicity of sodium xylene sulfonate to fathead minnow (*Pimephales promelas*) / 40422, 1992a

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 4.1_1300-72-7_2

Last Revised: 11-04-2005

Remarks: n/a

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 40.77%

Remarks: Substance tested are aqueous solutions; % purity equates to chemical content

Method

GLP: no

Report/Study Year: 1993

Report/Study Number: 13039.0393.6104.110

Method/Guideline Followed: EPA-TSCA 797-1300

Test Type: acute, static

Analytical Monitoring: no

Species: *Daphnia magna*, ≤ 24 hour old.

Exposure Period:

Value	Unit
48	hour(s)

Remarks: Number of daphnids: 5/beaker, 4 beakers/treatment.
Concentrations: Nominal: 130, 220, 360, 600 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Test conditions: Static without aeration; at 20 ± 2 °C in 250 mL glass vessels containing 200 mL of medium of hardness 160 mg/Ll ($CaCO_3$) and pH 8.2; 16 hour light, unfed.
Physical measurements: At 0, 24 and 48 hours: overall ranges for pH 8.0-8.2; O_2 87-89%; temperature 20 °C.
Observations: Immobility at 24 and 48 hours.

Results

Unit: mg /L

Results:

		Nominal Concentration (mg/L)					
Parameter	Time [hours]	0	130	220	360	600	1000
Immobility [%]	48	None					

48-hour EC50 >1000 mg/L (equivalent to > 408 mg/L active ingredient taking into account the 40.77% purity of the sample). No treatment related effects observed.

Remarks:

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. No GLP. No analyses

Reference

Source Reference: 49 Stepan Company, Northfield, Illinois, USA; Stepanate SXS ¨C Acute Toxicity to Daphnids (*Daphnia Magna*) under static conditions /13039.0393.6104.110, 1993b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Springborn Laboratories Inc., Wareham, Massachusetts, USA

Laboratory:
Print File Name: 4.2_1300-72-7_12
Last Revised: 11-04-2005
Remarks: n/a

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: 40%
Remarks: Substance tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes
Report/Study Year: 1992
Report/Study Number: 40424
Method/Guideline Followed: EPA-TSCA 797-1300
Test Type: static
Analytical Monitoring: no
Species: *Daphnia magna*, <24 hours old.

Exposure Period:

Value	Unit
48	hour(s)

Remarks: Statistical method: Binominal, moving average and probit analysis.
Number of daphnids: 10/beaker, 2 beakers/treatment.
Concentrations: Nominal: 100, 180, 320, 560 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Test conditions: Static without aeration; at 20 ± 2 °C in 250 mL glass vessels containing 200 mL of medium of hardness 150 mg/L ($CaCO_3$) and pH 8.3; 16 hours light, unfed.
Physical measurements: At 0 and 48 hours: overall ranges for pH 8.1-8.5; O_2 88-93%; temperature 20-21 °C.
Observations: Immobility/symptoms at 24 and 48 hours.

Results

Unit: mg/L

Results:

		Nominal concentration (mg/L)					
Parameter	Time [hours]	0	100	180	320	560	1000
Immobility [%]	48	None					

Symptoms	48	No treatment related effects

48-hour EC50 >1000 mg/L (equivalent to >400 mg/L active ingredient based upon 40% sample purity).

Remarks:

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. No analyses

Flag Critical study for SIDS endpoint

Reference

Source Reference: 39 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA; Acute Toxicity of sodium xylene sulfonate to *Daphnia Magna* / 40424, 1992d

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 4.2_1300-72-7_14

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1985

Report/Study Number: SDAHT06

Method/Guideline Followed: not indicated

Test Type: acute, static

Analytical Monitoring: n/a

Species: *Artemia sp.*

Exposure Period:

Value	Unit
48	hour(s)

Remarks: Nauplius life stage; synthetic sea water; static; pH 7.8-8.2; 20 °C. Mortality and loss of swimming ability were the endpoints considered.

Results

Results: 48-hour EC50 >400 mg/L

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 3 Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.2_1300-72-7_132

Last Revised: 6-21-2004

Remarks: n/a

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 40.77%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: no

Report/Study Year: 1993

Report/Study Number: 13039.0393.6105.430

Method/Guideline Followed: EPA-TSCA 797.1050

Analytical Monitoring: no

Species: Green algae (*Selenastrum capricornutum*).

Endpoint: Inhibition of cell growth

Exposure Period:

Value	Unit
96	hour(s)

Remarks: Initial cell concentration.: 10^4 cells/mL.
Three replicates per treatment.
Concentrations: Nominal: 16, 31, 63, 130, 250, 500 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected

for sample purity.
Test conditions: 125 mL flasks containing 50 mL of algal medium; temperature: 24 ± 1 °C; continuous illumination (3800-4600 lux); shaken (100 rpm).
Physical measurements: pH at 0 hour: 7.5-7.6 and at 96 hours: 9.6-10; temperature 24-25 °C.
Observations: Cell density at 0, 24, 48, 72 and 96 hours with a haemacytometer.

Results

Unit: mg/L

Results:

		Nominal Concentration (mg/L)							
Parameter	Time [hours]	0	16	31	63(A)	130(A)	250(A)	500(A)	1000(A)
Mean cell density [10^4 cells/mL]	0	1	1	1	1	1	1	1	1
	24	4	4	4	5	4	3	2	1
	48	12	8	12	10	12	6	7	4
	72	51	45	42	45	40	34	24	10
	96	102	96	97	76*	69*	59*	29*	11*
Inhibition [%] – area under curve	0-96	0	11	10	17	24	40	62	85
- growth rate	0-96	0	1	1	6	8	12	27	48

(A) Cell fragments, bloated cells and thin cell walls were observed as indicated.
* Statiscally significant reduction.

96-hour EC50 = 230 mg/L (95% CI 47-1200 mg/L)
96-hour NOEC = 31 mg/L

Growth measured during recovery period indicated that effects were algistatic and not algicidal.

Remarks:

- Recalculation of the EC50 by the reviewer based on area under the curve (using the 20% trimmed Spearman-Karber method) yielded an 96-hour EC50 value of 328 mg/L (95% CI 275-392 mg/L).
- *Minor remarks* Light intensity was only 3800-4600 lux (OECD 201 specifies 8000 lux). Since algal growth in controls was adequate, this did not affect the study outcome. The strong increase of pH over the test period was attributed to algal growth.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. No analyses, non-GLP

Flag Critical study for SIDS endpoint

Reference

Source Reference: 47 Stepan Company, Northfield, Illinois, USA. Stepanate SXS - Toxicity to the freshwater alga, *Selenastrum capricornutum* / 13039.0393.6105.430, 1993a

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	Springborn Laboratories Inc., Wareham, Massachusetts, USA
Print File Name:	4.3_1300-72-7_20
Last Revised:	11-04-2005
Remarks:	n/a

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2.A ACUTE ORAL TOXICITY

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: no
Report/Study Year: 1965
Report/Study Number: SDAHT08
Method/Guideline Followed: not indicated
Test type: n/a
Species: Rat
Strain: Sprague Dawley
Sex: male/female
Vehicle: n/a
Number of Animals per Dose: 5/sex/dose group
Doses: Single oral administration of 5000, 6300, 8000, 10000 and 12500 mg/kg bw, in distilled water; water controls; food was withheld 17-24 hours prior to dosing.
Remarks: Weights: males 102-139 g, females 89-121 g
Statistical method: Reed and Muench, 1938.
Observations:

- Mortality/clinical signs
- Body weights at dosing and after 1 and 2 weeks.
- Necropsy on all animals that died and selected survivors on day 15.

Results

Value: Oral LD50: 7200 mg/kg bw

Remarks:

Dose [mg/kg bw]		0		5000		6300		8000		10000		12500		DR	
Sex	Day	M	F	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	1-15	0/5	0/5	0/5	0/5	0/5	2/5	5/5	5/5	5/5	5/5	5/5	5/5	x	x
Clinical signs(A)	1-15	+	+	+	+	+	+	+	+	+	+	+	+		
Body weight	1-15	No treatment related effects													
Necropsy(B)	15						+	+	+	+	+	+	+		

(A)On day 1 lethargy, diarrhoea, ptosis, lachrymation and piloerection were observed among animals.

(B)Findings in the animals that died included slight pulmonary inflammation, gastrointestinal inflammation and haemorrhage and mild liver changes.

- An additional test was performed on the impurities that were extracted. This test gave a LD50 for these impurities of >10000 mg/kg. The LD50 reported in the main study can therefore be attributed to effects of the test substance. However, since the amount of active ingredient in the test substance is not known, no correction on the LD50 could be made.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Purity of the test substance was not known.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 16 Marchon Products Ltd., Whitehaven, Cumberland, UK. Acute oral toxicity of samples A.8969[1] and A.8970[2] in the rat / 1379/65/297. 1965

Other References: 3 Albright & Wilson Ltd, France, IUCLID Data Sheet for Sodium Xylenesulphonate, 2000

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Huntingdon Research Center, Huntingdon, UK

Print File Name: 5.1.1_1300-72-7_29

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	40%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	no
Report/Study Year:	1975
Report/Study Number:	202098
Method/Guideline Followed:	not indicated
Test type:	n/a

Species:	Rat
Strain:	COX-SD
Sex:	male/female
Vehicle:	none
Number of Animals per Dose:	5/sex/dose group
Doses:	Single oral administration of 10020, 12620, 15890, 20000 and 25180 mg/kg bw, (dosing volume 9-21 mL/kg); no controls; feeding *ad libitum* (food was withheld overnight prior to dosing).
Remarks:	Weight: 195-334 g Age – not provided Observations:

- Mortality/clinical signs several times on day 1 and daily until day 15.
- Body weights on day 1 and 15.
- Necropsy on animals that died and survivors on day 15.

Results

Value: Oral LD50 = 16200 mg/kg bw

Remarks:

Dose [mg/kg bw] effect		10020		12620		15890		20000		25180		DR	
Sex	Day	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	0-15	0/5	0/5	0/5	0/5	2/5	0/5	4/5	4/5	4/5	5/5	5/5	x
Clinical signs(A)	0-15	+	+	+	+	+	+	+	+	+	+	+	x
Body weight	0-15	No treatment related effects											
Necropsy(B)	15				+		+	+	+	+	+	x	x

(A)Symptoms consisted of weakness, oily ventral skin and hair and prostration.
(B)Findings consisted of severe congestion of the liver, kidneys, adrenal gland and gastrointestinal tract in the animals that died and slight to moderate congestion of the adrenal glands of survivors.
DR = dose related. (should this be a sentence instead of columns?)

Oral LD50 16200 mg/kg bw is equivalent to 6500 mg/kg active ingredient considering the 40% purity of substance.

Minor remark. The evaluation of body weight is hampered, because no control group was included in the study design

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Results not reported on individual animals.

Reference

Source Reference: 4 Continental Oil Company, Ponca City, Oklahoma, USA. Acute oral Toxicity (LD50) in Rats / 202098, 1975a

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	Scientific Associates Inc., St. Louis, Missouri, USA
Print File Name:	5.1.1_1300-72-7_30
Last Revised:	11-04-2005
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	40% aqueous concentration

Method

GLP:	n/a
Report/Study Year:	1978
Report/Study Number:	SDAHT07
Method/Guideline Followed:	not indicated
Test type:	n/a
Species:	Rat
Remarks:	No details provided

Results

Value: LD50 = 16,200 mg/kg

Remarks: 95% confidence limit of 14,000-18,800 mg/kg

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name:	5.1.1_1300-72-7_31
Last Revised:	6-22-2004
Remarks:	This is likely the same study reported in (4) Continental Oil Company, Ponca City, Oklahoma, USA. Acute oral Toxicity (LD50) in Rats / 202098, 1975a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	n/a
Remarks:	40% aqueous solution

Method

GLP:	n/a
Report/Study Year:	1972
Report/Study Number:	SDAHT09
Method/Guideline Followed:	n/a
Test type:	n/a
Species:	Albino Rat
Strain:	Wistar
Sex:	male
Vehicle:	n/a
Number of Animals per Dose:	10
Doses:	5000 mg/kg
Remarks:	Weight: 200-250 g aqueous solution at pH 7.6 and 9.4

Results

Value: LD50 >5000 mg/kg

Remarks: one death at pH 7.6

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 53 Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data.

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	5.1.1_12068-03-0_122
Last Revised:	6-22—2004
Remarks:	n/a

5.2.B ACUTE INHALATION TOXICITY

Acute inhalation toxicity data are available for CAS numbers 12068-03-0, 26447-10-9, and 28348-53-0 (32073-22-6).

5.2.C ACUTE DERMAL TOXICITY

Acute dermal toxicity data are available for CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

5.3.A SKIN IRRITATION

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	40% aqueous solution

Method

GLP:	no
Report/Study Year:	1975
Report/Study Number:	202098-D
Method/Guideline Followed:	not indicated
Analytical Monitoring:	n/a
Species:	Rabbit
Strain:	New Zealand White
Vehicle:	n/a
Number of Animals:	6 (sex not indicated).
Concentration:	n/a
Exposure:	Application of 0.5 ml test substance (no vehicle) on 2.5x2.5 cm of the clipped dorsal skin in two areas (intact and abraded) under occlusion for 24 hours.
Remarks:	Observations: Skin observations at 24, 48 and 72 hours after application using Draize method.

Results

Result:	slightly irritating
Primary Dermal Irritation Index (PDII):	1.4
Remarks:	The results of tests with abraded skin and intact skin are comparable. The scores shown below apply to both conditions. The PDII is an average of the two conditions.

Animal	1	2	3	4	5	6

Time	E	O	E	O	E	O	E	O	E	O	E	O
24 h	1	1	1	1	1	1	3	2	1	1	1	1
48 h	0	0	1	0	1	0	3	2	1	0	1	0
72 h	0	0	0	0	0	0	2	0	0	0	0	0

E=erythema and escher
O=oedema

Since skin effects were still present in one animal at the 72 hour observation, the test should have been extended for an additional period (maximum up to 21 days).

Minor remarks. No information on the time of clipping of the fur was provided. No information on body weights was present. The 24-h exposure period represents a worst case scenario.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Effects present at the last observation time. The purity of the substance is unknown.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 5. Continental Oil Company, Ponca City, Oklahoma, USA. Dermal Irritation tests in Rabbits / 202098. 1975b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Scientific Associates Inc., St. Louis, Missouri, USA

Print File Name: 5.2.1_1300-72-7_46

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: not indicated

Remarks: 40% solution

Method

GLP: n/a

Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Species: rabbits
Strain: New Zealand albino
Vehicle: n/a
Number of Animals: n/a
Concentration: n/a
Exposure: Applied to both intact and abraded skin.
Remarks: n/a

Results

Result: slightly irritating
Primary Dermal Irritation Index (PDII): n/a
Remarks: "As defined in the Federal Hazard Substance Act (FHSA), the substance was found not to be a primary irritant"

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 5.2.1_1300-72-7_51
Last Revised: 6-22-2004
Remarks: n/a

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1981
Report/Study Number: SDAHT03
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Species: rabbit
Vehicle: n/a
Number of Animals: n/a
Concentration: 40% solution
Exposure: Applied to both intact and abraded skin.
Remarks: n/a

Results

Result: slightly irritating
Primary Dermal Irritation Index (PDII): n/a
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 52. Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. >= 1981

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: Overview of available data
Print File Name: 5.2.1_1300-72-7_53
Last Revised: 6-22-2004
Remarks: n/a

5.3.B EYE IRRITATION

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: n/a
Species: Rabbit
Strain: New Zealand albino
Vehicle: n/a
Number of Animals: 6
Dose: n/a
Remarks: 40% solution; instilled into the conjunctival sac and the treated eyes were not rinsed.

Results

Result: slightly irritating
Remarks: Slight to moderate effects within 24 hours, but cleared at 72 hours except for a slight erythmea.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary Literature.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.2_1300-72-7_52
Last Revised: 11-04-2005
Remarks: n/a

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: Not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1981
Report/Study Number: SDAHT03
Method/Guideline Followed: not indicated

Species: Rabbit
Vehicle: n/a
Number of Animals: 6
Dose: n/a
Remarks: 40% solution

Results

Result: slightly irritating
Remarks: Slight to moderate effects within 24 hours; recovered at 72 hours except for redness.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 52. Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. >= 1981

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.2_1300-72-7_54
Last Revised: 6-22-2004
Remarks: n/a

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: Not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1972
Report/Study Number: SDAHT09
Method/Guideline Followed: n/a
Species: Albino Rabbit
Vehicle: n/a
Number of Animals: 6 per dose
Dose: n/a
Remarks: 40% aqueous solution; at pH 7.6 and 9.4

Results

Result: slightly irritating

Remarks: Considered a minimal irritant according to Federal Hazardous Substances Act regulations, Section 191.12.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 53. Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 5.2.2_1300-72-7_125

Last Revised: 6-22-2004

Remarks: n/a

5.4 SENSITIZATION

Skin sensitization data are available for CAS numbers 12068-03-0, and 28348-53-0 (32073-22-6).

5.5 REPEATED DOSE TOXICITY

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 65%

Remarks: purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP: no

Report/Study Year: 1998

Report/Study Number: 98-3380

Method/Guideline Followed: not indicated

Analytical Monitoring: At study start from all concentrations by HPLC

Test Type: n/a

Species: Rat, age 5 weeks, mean weight 93-114 g.

Strain: F344/N

Sex: Males/females

No. of animals 5 per sex per dose group

Route of Administration:	Dermal (clipped skin)
Exposure Period:	17 days
Doses:	5, 15, 44, 133 and 400 mg/ml (vehicle water, volume applied 0.3 ml) which averaged approximately 10, 30, 90, 260 and 800 mg a.i./kg bw for males and 13, 40, 120, 330 and 1030 mg a.i./kg bw for females based upon 65% purity of substance; solutions/suspensions were prepared twice during the study; feeding *ad libitum*.
Control Group:	Vehicle controls
Frequency of Treatment:	5 days/week
Post Exposure Observation Period:	n/a
Remarks:	Stat. method Kaplan-Meier. Observations Mortality/ clinical signs twice daily. Body weights on day 1, 8 and at termination. Necropsy at termination Heart, right kidney, liver, lungs, right testis and thymus weights. Histopathology of the skin and gross lesions.

Results

Value: NOAEL = 400 mg/ml which equals 1030 mg/kg bw active ingredient (a.i.)

Results: Analyses: Mean measured concentrations 99-104% of nominal; stability in 50% ethanol at room temperature in dark (4 mg/ml and 75 mg/ml) for 21 and 29 days respectively confirmed.

Dose [mg/ml] effect		0		5		15		44		133		400		DR	
Sex	Day	M	F	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	17	None													
Clinical signs(A)	1-17			+	+	+	+	+	+	+	+	+	+		
Body weight gain	1-17	No treatment related effects													
Necropsy(B)	17	No test substance related effects													
Organ weights - liver	17									ic^r	ic^r	ic^r	ic^r	x	x

(A) Signs included tan or brown discolouration of the skin and crusty white deposits at the application site.
(B) Skin lesions related to clipping were observed among animals.
DR = dose related (indicated with an "x")
ic = significant increase
r = relative to body weight

Remarks:
1. The effects on relative liver weights were considered to be of unknown toxicological relevance.
2. The studies are used as dose range finding studies for a carcinogenicity study. Therefore the number of endpoints was limited.

3. The analyses for stability were performed in 50% ethanol. This is not the vehicle used in this study. Stability in water may differ.

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions. Limited report (note 2), no analyses for stability in water (note 3).

Reference

Source Reference:	51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (Cas No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA
Print File Name:	5.4_1300-72-7_78
Last Revised:	6-29-2004
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	65%
Remarks:	purity 65% (11.5% ortho, 38% meta and 15.5% para)

Method

GLP:	no
Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	not indicated
Analytical Monitoring:	At study start from all concentrations by HPLC
Test Type:	n/a
Species:	Mouse, age 6 weeks, mean weight 18-24 g.
Strain:	B6C3F1
No. of animals	5 per sex per dose group

Sex:	Male/female
Route of Administration:	Dermal (to clipped skin)
Exposure Period:	17 days
Doses:	5, 15, 44, 133 and 400 mg/l (vehicle water, volume applied 0.1 ml) which averaged approximately 20, 60, 190, 540 and 1600 mg a.i./kg bw for males and 26, 80, 220, 680 and 2000 mg a.i./kg bw for females taking into consideration the 65% purity of the substance. Solutions/suspensions were prepared twice during the study; feeding *ad libitum*.
Control Group:	Vehicle controls
Frequency of Treatment:	5 days per week
Post Exposure Observation Period:	n/a
Remarks:	Stat. method: Kaplan-Meier.
	Observations: Mortality/ clinical signs twice daily. Body weights on day 1, 8 and at termination. Necropsy at termination Heart, right kidney, liver, lungs, right testis and thymus weights. Histopathology of the skin and gross lesions.

Results

Value: NOAEL = 400 mg/ml which equals 2000 mg/kg bw active ingredient (a.i.)

Results: Mean measured concentrations 99-104% of nominal; stability in 50% ethanol at room temperature in dark (4 mg/ml and 75 mg/ml) for 21 and 29 days respectively confirmed.

Dose [mg/ml] effect		0		5		15		44		133		400		DR	
Sex	Day	M	F	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	17	None													
Clinical signs(A)	1-14									+		+	+		
Body weight gain	1-17	No treatment related effects													
Necropsy(B)	17	No test substance related effects													
Organ weights - liver	17						ic^{r}		ic^{r}		ic^{r}	ic^{r}		x	x

(A) Signs included crusty white deposits at the application site.
(B) Skin lesions related to clipping were observed among animals.
DR = dose related (indicated with an "x")
ic = significant increase
r = relative to body weight

Remarks:
1. The effects on organ weights (especially liver) were considered to be of unknown toxicological relevance.
2. The studies are used as dose range finding studies for a carcinogenicity study. Therefore the number of endpoints was limited.

3. The analyses for stability were performed in 50% ethanol. This is not the vehicle used in this study. Stability in water may differ.

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions. Limited report (note 2 in 'Results *Remarks*'), no analyses for stability in water (note 3 in 'Results *Remarks*').

Reference

Source Reference:	51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (Cas No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA
Print File Name:	5.4_1300-72-7_79
Last Revised:	6-29-2004
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	65%
Remarks:	purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP:	yes
Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	Not indicated; resembles OECD 411
Analytical Monitoring:	At the beginning, mid and end of the study period from all concentrations by HPLC
Test Type:	n/a
Species:	Mouse, age 7 weeks, mean weight males 25-26 g, females 19-20 g.
Strain:	B6C3F1
Sex:	Males/females

No. of animals	10 per sex per dose group
Route of Administration:	Dermal (to clipped skin)
Exposure Period:	13 weeks
Doses:	5, 15, 44, 133 and 400 mg/ml (vehicle 50% ethanol, volume applied 0.1 ml) which averaged approximately 17, 50, 140, 440 and 1300 mg a.i./kg for males and 20, 60, 170, 540 and 1620 mg a.i./kg for females taking into consideration the 65% purity of the substance; solutions/suspensions were prepared every 2 weeks; feeding *ad libitum*.
Control Group:	Vehicle controls
Frequency of Treatment:	5 days per week
Post Exposure Observation Period:	n/a
Remarks:	Stat. method Kaplan-Meier. Observations As per OECD 411 with the exception of clinical signs recorded weekly, no food consumption, no ophthalmoscopy, clinical chemistry (performed only in rats, no sodium, potassium, chloride, phosphorus and glucose) and histopathology of the skin at all dose levels.

Results

Value: NOAEL (female) = 133 mg/ml which equals 530 mg/kg bw active ingredient (a.i.) based on epidermal hyperplasia.

NOAEL (male) = 133 mg/ml which equals 440 mg/kg bw active ingredient (a.i.) based on epidermal hyperplasia.

Results: Mean measured concentrations 99-106% of nominal; stability in 50% ethanol at room temperature in dark (4 mg/ml and 75 mg/ml) for 21 and 29 days resp. confirmed.

Dose [mg/ml] effect	0		5		15		44		133		400		DR	
Sex	M	F	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	None													
Clinical signs	None													
Body weight gain											ic			
Haematology	Not performed													
Clinical biochemistry	Not performed													
Organ weight														
Kidney			ic^{r}		ic^{ar}		ic^{ar}				ic^{a}			
Necropsy	No treatment related effects													
Histopathology														
Epidermal hyperplasia of the application site											+	+		

DR = dose related (indicated with an "x")
ic = significant increase
a = absolute to body weight
r = relative to body weight

Remarks:
1. The effects on kidney weights in males were inconsistent, not dose related and were therefore not considered to be of biological relevance.
2. The histopathological examinations were conducted, but the results were not reported in the original study.
3. The studies are used as dose range finding studies for a carcinogenicity study. Therefore the number of endpoints was limited

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Limited report (note 3).

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (Cas No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA

Print File Name: 5.4_1300-72-7_81

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 65%

Remarks: purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP: yes

Report/Study Year: 1998

Report/Study Number: 98-3380

Method/Guideline not indicated; resembles OECD 411

Followed:

Analytical Monitoring:	At the beginning, mid and end of the study period from all concentrations by HPLC
Test Type:	n/a
Species:	Rat, age 6 weeks, mean weight males 133-147 g, females 99-110 g.
Strain:	F344/N
Sex:	Males/females
No. of animals	10/sex/dose group (additional 10/sex/dose group for haematology and clinical chemistry on day 5 and 21).
Route of Administration:	Dermal (to clipped skin)
Exposure Period:	13 weeks
Doses:	5, 15, 44, 133 and 400 mg/ml (vehicle 50% ethanol, volume applied 0.3 ml) which averaged approximately 6, 20, 60, 170 and 500 mg a.i./kg for males and 10, 30, 90, 260 and 800 mg a.i./kg for females taking into consideration the 65% purity of the substance; solutions/suspensions were prepared every 2 weeks; feeding *ad libitum*.
Control Group:	Vehicle controls
Frequency of Treatment:	5 days per week
Post Exposure Observation Period:	n/a
Remarks:	Stat. method: Kaplan-Meier. Observations: As per OECD 411 with the exception of clinical signs recorded weekly, no food consumption, no ophthalmoscopy, clinical chemistry (performed only in rats, no sodium, potassium, chloride, phosphorus and glucose) and histopathology of the skin at all dose levels.

Results

Value: NOAEL = 400 mg/ml which equals 800 mg/kg bw active ingredient (a.i.)

Results: Mean measured concentrations 99-106% of nominal; stability in 50% ethanol at room temperature in dark (4 mg/ml and 75 mg/ml) for 21 and 29 days resp. confirmed

Dose [mg/ml] effect	0		5		15		44		133		400		DR	
Sex	M	F	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	None													
Clinical signs			+	+	+	+	+	+	+	+	+	+		
Body weight gain	No treatment related effects													
Haematology	No treatment related effects													
Clinical biochemistry														
ALAT day 5							ic		ic		ic			

Organ weight																								
Lung								dc[a]			dc[a]													
Liver								dc[ar]			dc[ar]			dc[ar]			x						
Necropsy	No treatment related effects																							
Histopathology																								
Epidermal hyperplasia of the application site[1]					+									+										

[1]Signs consisted of brown discolouration of the skin at application site.
DR = dose related (indicated with an "x")
ic = significant increase
dc = significant decrease
a = absolute to body weight
r = relative to body weight

Remarks:
1. The effect on liver weights was not accompanied by histopathology changes and were considered not to be of biological relevance.
2. An effect on liver enzymes was only reported in male rats after 5 days of exposure. Since no effects were reported in females and at later measurements, no toxicological significance was attributed to this effect.
3. The histopathological examinations were conducted, but the results were not reported in the original study.
4. The studies are used as dose range finding studies for a carcinogenicity study. Therefore the number of endpoints was limited.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Limited report (note 3 in 'Results *Remarks*').

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (Cas No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA

Print File Name: 5.4_1300-72-7_80

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	Not given; stated that the major component was the chemical. Assume 100%
Remarks:	Compound reported as stable

Method

GLP:	Not indicated but appears to meet the intent
Report/Study Year:	1980
Report/Study Number:	Gulf Coast Research Institute No. 410-798
Method/Guideline Followed:	Not indicated; resembles OECD 408
Analytical Monitoring:	Analysis of the compound/feed mixture at all levels was performed once during the study
Test Type:	n/a
Species:	Rat, age 57 days, weight range males 144-174 g, females 116-144 g.
Strain:	Fischer 344
Sex:	Males/females
No. of animals	10 per sex per dose group
Route of Administration:	Oral in diet
Exposure Period:	13 weeks
Doses:	0, 0.125, 0.25, 0.5, 1.0 and 2.0% in the diet
Control Group:	Basal diet with no added test material
Frequency of Treatment:	Fed *ad libitum*; diets prepared weekly
Post Exposure Observation Period:	n/a

Remarks:

Test material	Identified as C55403, Lot No. 3835, supplied by Witco Chemical Corporation
Observations	Individual animal weights and clinical signs recorded weekly. Food consumption weekly. Pharmaco-toxic signs and mortality twice daily. Gross pathology at sacrifice. Histopathology performed on all control and high level animals. Tissue examinations include: blood smear, lymph nodes, salivary gland, sternebrae/femur/vertebrae including marrow, thyroid, parathyroids, small intestine, colon, liver, prostate, testes, ovaries, lungs and mainstem bronchi, mammary gland, heart, esophagus, stomach, uterus, brain, thymus, trachea, pancreas, spleen, kidneys, adrenals, urinary bladder, pituitary, spinal cord, eyes.

Results

Value: NOEL (female) = 1561 mg/kg bw per day

NOEL (male) = 1429 mg/kg bw per day

Results:

Dose [percent in diet]	0		0.125		0.25		0.5		1.0		2.0	
Actual mean dose admin. (mg/kg/day)	0	0	89	98	179	195	357	390	715	781	1429	1561
Sex	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	No treatment related effects											
Clinical signs	No treatment related effects											
Food consumption	No treatment related effects											
Body weight	dc* No treatment related effects at other doses											
Haematology	Not performed											
Clinical biochemistry	Not performed											
Organ weight	Not performed											
Necropsy	No treatment related effects											
Histopathology	No treatment related effects											
Gross or microscopic lesions	No treatment related effects											

Remarks:
1. * Reduction in female body weight gain of 17.7% at 1% dose
2. NOELs based on reported body weight and feed intake data and assuming 100% purity of test compound
3. The study was used to determine the Maximum Tolerated Dose (MTD) to be used in a chronic toxicity bioassay. No treatment related effects were observed at the highest administered dose.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with some restrictions. Purity not reported and no indication of organ weight measurements.

Reference

Source Reference: 54. Tracor Jitco, Inc. Subcontract No. 76-36-106001; GSRI No. 410-798. A subchronic test of xylene sulfonic acid sodium salt (C55403) in B6C3F1 mice and Fischer 344 rats. March 21, 1980.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Gulf South Research Institute, Louisiana, USA

Print File

Name:
Last Revised: 3-21-2005
Remarks: Study sponsored by the U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program.

Test Substance

CAS Number: 1300-72-7
Identity: Xylene sulfonic acid, sodium salt
Purity: Not given; stated the major component was the chemical. Assume 100%
Remarks: Compound reported as stable

Method

GLP: Not indicated but appears to meet the intent
Report/Study Year: 1980
Report/Study Number: Gulf Coast Research Institute No. 410-798
Method/Guideline Followed: Not indicated; resembles OECD 408
Analytical Monitoring: Analysis of the compound/feed mixture at all levels was performed once during the study
Test Type: n/a
Species: Mouse, age 57 days, weight range males 20-30 g, females 18-24 g.
Strain: Charles River B6C3F1
Sex: Males/females
No. of animals 10 per sex per dose group
Route of Administration: Oral in diet
Exposure Period: 13 weeks
Doses: 0, 0.125, 0.25, 0.5, 1.0 and 2.0% in the diet
Control Group: Basal diet with no added test material
Frequency of Treatment: Fed *ad libitum*; diets prepared weekly
Post Exposure Observation Period: n/a
Remarks:

Test material	Identified as C55403, Lot No. 3835, supplied by Witco Chemical Corporation
Observations	Individual animal weights and clinical signs recorded weekly. Food consumption weekly. Pharmaco-toxic signs and mortality twice daily. Gross pathology at sacrifice. Histopathology performed on all control and high level animals. Tissue examinations include: blood smear, lymph nodes, salivary gland,

sternebrae/femur/vertebrae including marrow, thyroid, parathyroids, small intestine, colon, liver, prostate, testes, ovaries, lungs and mainstem bronchi, mammary gland, heart, esophagus, stomach, uterus, brain, thymus, trachea, pancreas, spleen, kidneys, adrenals, urinary bladder, pituitary, spinal cord, eyes.

Results

Value: NOEL (female) = 2467 mg/kg bw per day

NOEL (male) = 2439 mg/kg bw per day

Results:

Dose [percent in diet]	0		0.125		0.25		0.5		1.0		2.0	
Actual mean dose admin. (mg/kg/day)	0	0	152	154	305	308	610	617	1220	1234	2439	2467
Sex	M	F	M	F	M	F	M	F	M	F	M	F
Mortality	No treatment related effects											
Clinical signs	No treatment related effects											
Food consumption	No treatment related effects											
Body weight	i	d	i	i	i	i	i	d	i	d		
Haematology	Not performed											
Clinical biochemistry	Not performed											
Organ weight	Not performed											
Necropsy	No treatment related effects											
Histopathology	No treatment related effects											
Gross or microscopic lesions	No treatment related effects											

Remarks:

1. NOELs based on reported body weight and feed intake data and assuming 100% purity of test compound. Body weights varied widely in both sexes. Effects on body weight in females as compared to controls were -2, +0.4, +3, -4 and -5 % at the doses administered. Body weights of all male groups increased (<5%) as compared to controls at the end of the study.
2. The study was used to determine the Maximum Tolerated Dose (MTD) to be used in a chronic toxicity bioassay. No treatment related effects were observed at the highest administered dose.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with some restrictions. Purity not reported and no indication of organ weight measurements.

Reference

Source 54. Tracor Jitco, Inc. Subcontract No. 76-36-106001; GSRI No. 410-798. A

Reference: subchronic test of xylene sulfonic acid sodium salt (C55403) in B6C3F1 mice and Fischer 344 rats. March 21, 1980.

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	Gulf South Research Institute, Louisiana, USA
Print File Name:	
Last Revised:	3-21-2005
Remarks:	Study sponsored by the U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program.

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	not indicated; see remarks
Remarks:	Purity is reported as 93% in Ref. 3 (IUCLID) and confirmed by Huntsman company representative via e-mail to Hydrotropes Consortium on 12-6-2004.

Method

GLP:	no
Report/Study Year:	1969
Report/Study Number:	R2822
Method/Guideline Followed:	not indicated; resembles OECD 408
Analytical Monitoring:	n/a
Test Type:	n/a
Species:	Rat, males 45-64 g, females 41-60 g.
Strain:	Wistar
Sex:	Male/female
No. of animals	15 per sex per dose group
Route of Administration:	Diet
Exposure Period:	13 weeks
Doses:	0, 0.2, 1.0 and 5.0 % in diet; diets were prepared once a fortnight.
Control Group:	yes
Frequency of Treatment:	diet
Post Exposure	n/a

Observation Period:

Remarks:

Test material	Halvopon OR which is a powder grade, with an active spec (i.e., solids minus sulphate) of 93% minimum.
Observations	Mainly as required by OECD 408 with the exception of: clinical signs, functional observations, ophthalmoscopy, haematology (no platelets and blood clotting potential) and clinical chemistry (samples from 10 animals/group; no sodium, potassium and cholesterol).

Results

Value: NOAEL (male) >3800 mg/kg bw/day = 3534 mg a.i./kg bw/day calculated using 93% active ingredient
NOAEL (female) = 820 mg/kg bw/day = 763 mg a.i./kg bw/day calculated using 93% active ingredient (based on relative weight loss in spleen)

Results:

Dose (% in diet)	0		0.2		1.0		5.0		DR	
Actual mean dose admin. (mg/kg/day)	0	0	140	160	710	820	3800	4400		
Actual mean dose admin. (mg a.i./kg/day) using 93% active ingredient	0	0	130	149	660	763	3534	4092		
Sex	M	F	M	F	M	F	M	F	M	F
Mortality	None									
Clinical signs	Not reported									
Body weight gain							d	d		
Food consumption[A]	No treatment related effects									
Water consumption							i	i		
Haematology										
RBC week 6							dc	dc		
Clinical biochemistry										
SGOT							d	dc	x	x
Glucose			dc		dc		dc			
Glucose-6-phosphatase							i			
Glucose-6-phosphate dehydr.							d	d		
Urinalysis										
Specific gravity								dc		
Protein week 13	i		i		i		i			
Organ weight										
Spleen								dc^r		x
Necropsy[B]	No treatment related effects									
Histopathology[C]										
Increase and enlargment of Kupfer cells (occasionally with iron pos. granules)							+	+		

(A) Food intake at 5.0% was decreased during the first two weeks of the study, but recovered to control levels during the rest of the study.
(B) Abnormalities found among animals were proteinaceous plugs in urinary bladder, slight hydronephrosis and small, greyish depressed areas in the lungs, distended uterine horns filled with watery fluid and a pale liver.
(C) The following organs were examined for histopathological changes: hearts, spleen, liver, kidney, brain, testicle/ovary, thymus, pituitary, thyroid and adrenal.
Histopathologically findings were essentially negative. A few abnormalities considered not treatment related were as following:
- a pale liver in one male control rat
- distended uterine horns filled with liquid in one female at 0.2% and 1% test substance
- haemorrhagic foci in the thymus of one female animal at 1% test substance.

DR = dose related (indicated with an "x")
i = increase
d = decrease
dc = significant decrease
r = relative to body weight (12% decrease)

Remarks:

1. The age of the animals used in the study was not indicated. Based on weight rats must have been <6 weeks at study initiation. This may influence the results of the study. OECD 408 requires young adults.
2. The increased protein level seen in the urine of males at all treatment groups may be related to the presence of proteinaceous plugs in urinary bladder, which is stated to be a common finding in rats of this strain. Since no individual data were presented, this relationship could not be checked by the reviewer.
3. The decreased glucose level (versus the control) seen in males of all treatment groups was not dose dependent and was attributed, by the authors, to the unusually high glucose level in the control.
4. Diet was prepared every 14 days. No analyses of accuracy of preparation and of stability under storage conditions were performed.
5. Body weight was determined every two weeks. The actual test substance intake is stated to be 700 mg/kg at the 1.0% level. The actual test substance intake data in the table above are calculated by the reviewer and are based on the mean body weight measured at the end of the two week period. This is considered to be an underestimation of true test substance intake. The NOAEL found considered to be a worst case estimation.

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions. Animals too young (note 1) and no analyses (note 4).
Flag	Critical study for SIDS endpoint

Reference

Source Reference: 2. Albright & Wilson Ltd. (Marchon Division), Whitehaven, Cumberland, UK. Subchronic (90-day) toxicity study with Halvopon OR in albino rats / R 2822. 1969

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	TNO, Zeist, The Netherlands
Print File Name:	5.4_1300-72-7_82
Last Revised:	11-04-2005
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	Not given
Remarks:	Compound reported as stable

Method

GLP:	Not indicated but appears to meet the intent
Report/Study Year:	1979
Report/Study Number:	Gulf Coast Research Institute No. 412-798
Method/Guideline Followed:	Not indicated
Analytical Monitoring:	Analysis of the compound/feed mixture was not required for this range finding study
Test Type:	14-day range finding
Species:	Mouse, weight range males 22-27 g, females 17-23 g.
Strain:	Charles River B6C3F1
Sex:	Males/females
No. of animals	5 per sex per dose group
Route of Administration:	Oral in diet
Exposure Period:	14 days
Doses:	0, 0.25, 0.5, 1.0, 2.0 and 4.0% in the diet
Control Group:	Basal diet with no added test material
Frequency of Treatment:	Fed *ad libitum*
Post Exposure Observation Period:	n/a
Remarks:	Test material: Identified as C55403, Lot No. 3835, supplied by Witco Chemical Corporation
	Observations: Individual animal weights and food consumption recorded weekly. Observed twice daily for signs of intoxication and

mortality. Gross pathology at sacrifice.

Results

Value: Recommended of 2% maximum dose level in subchronic test

Results: No mortalities; no clinical signs of distress or toxicity and no gross lesions. Body weight changes indicated a possible toxic effect in both sexes at 1, 2 and 4% diets. Males gained less weight as compared to controls at 1, 2 and 4% dose levels (reduction in body weight gain is 2, 2 and 6% of controls). Females gained less than the controls at the 1, 2 and 4% dose levels (reduction in body weight gains is 1, 1 and 3% of controls). Both sexes at the 0.25 and 0.5% levels outgained their controls (2, 3% in males and 1, 4% in females). Overall the reductions in body weight gain are <10% compared to controls. Appears to be an initial palatability problem with the mice consuming considerably more feed in the second week than in the first week.

Remarks: None

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions.

Reference

Source Reference: 55. Tracor Jitco, Inc. Subcontract No. 76-36-106002; GSRI No. 412-798. A repeated dose test of xylene sulfonic acid sodium salt (C55403) in B6C3F1 mice and Fischer 344 rats. July 26, 1979.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Gulf South Research Institute, Louisiana, USA

Print File Name:

Last Revised: 3-21-2005

Remarks: Study sponsored by the U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program.

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: Not given

Remarks: Compound reported as stable

Method

GLP: Not indicated but appears to meet the intent

Report/Study Year: 1979

Report/Study Number: Gulf Coast Research Institute No. 412-798

Method/Guideline Followed:	Not indicated
Analytical Monitoring:	Analysis of the compound/feed mixture was not required for this range finding study
Test Type:	14-day range finding
Species:	Rat, range males 92-138 g, females 78-112 g.
Strain:	Fischer 344
Sex:	Males/females
No. of animals	5 per sex per dose group
Route of Administration:	Oral in diet
Exposure Period:	14 days
Doses:	0, 0.25, 0.5, 1.0, 2.0 and 4.0% in the diet
Control Group:	Basal diet with no added test material
Frequency of Treatment:	Fed *ad libitum*
Post Exposure Observation Period:	n/a
Remarks:	Test material: Identified as C55403, Lot No. 3835, supplied by Witco Chemical Corporation
	Observations: Individual animal weights and food consumption recorded weekly. Observed twice daily for signs of intoxication and mortality. Gross pathology at sacrifice.

Results

Value: Recommended of 2% maximum dose level in subchronic test

Results: Six male rat deaths (2 at 2% and 4 at 4%) and four female rat deaths (1 each at 0.5, 1, 2, and 4%). Reduction in body weight gain in males at 1% and 2% dose levels were 3 and 19% as compared to controls. Females outgained the controls except for the 4% level where the gain was 7% less than controls. They were observed scratching their feed out of their dishes beginning about day 5 indicating a probable palatability problem. Some refused the food until they became thin and even died. Pathology did not find any compound related lesions at any dose level.

Remarks: None

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions.

Reference

Source Reference: 55. Tracor Jitco, Inc. Subcontract No. 76-36-106002; GSRI No. 412-798. A repeated dose test of xylene sulfonic acid sodium salt (C55403) in B6C3F1 mice and Fischer 344 rats. July 26, 1979.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory:	Gulf South Research Institute, Louisiana, USA
Print File Name:	
Last Revised:	3-21-2005
Remarks:	Study sponsored by the U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program.

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	Not given
Remarks:	Compound reported as stable

Method

GLP:	Not indicated but appears to meet the intent
Report/Study Year:	1980
Report/Study Number:	Gulf Coast Research Institute No. 410-798
Method/Guideline Followed:	Not indicated
Analytical Monitoring:	Analysis of the compound/feed mixture was not required
Test Type:	14-day range finding
Species:	Rat, range males 134-163 g, females 110-126 g.
Strain:	Fischer 344
Sex:	Males/females
No. of animals	5 per sex per dose group
Route of Administration:	Oral in diet
Exposure Period:	14 days
Doses:	0, 1.0, 2.0 and 4.0% in the diet
Control Group:	Basal diet with no added test material
Frequency of Treatment:	Fed *ad libitum*
Post Exposure Observation Period:	n/a
Remarks:	Test material: Identified as C55403, Lot No. 3835, supplied by Witco Chemical Corporation
	Observations: Individual animal weights recorded weekly. Observed twice daily for pharmacotoxic signs and mortality. Food consumption recorded weekly and gross pathology at sacrifice.

Results

Value: Maximum Tolerated Dose of 2%

Results: No unscheduled deaths at any levels. Males in the 1%, 2% and 4% groups gained less weight than the controls (reductions in body weight gains being 5, 4, and 17%, respectively). Females in the 1%, 2% and 4% groups gained less than controls (reduction in body weight gains being 2, 1.6 and 4.6% respectively). Both sexes were observed scratching feed out of their feeders during the last eight days of the test indicating a possible taste acceptance problem. This correlates with the reduced weight gains. There were no signs indicative of toxicity or physical distress observed. No lesions were found at necropsy.

Remarks: This test was conducted because of the total lack of clinical or histological signs of toxicity found during the 90-day subchronic test and because the earlier 14-day repeated dose, range finding test with rats had resulted in 5/10 deaths at 4%, 3/10 at 2% and 1/10 at 1%.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions.

Reference

Source Reference: 56. Tracor Jitco, Inc. Subcontract No. 76-36-106002; GSRI No. 410-798. A repeated dose test rerun of xylene sulfonic acid sodium salt (C55403) in Fischer 344 rats. May 19, 1980

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Gulf South Research Institute, Louisiana, USA

Print File Name:

Last Revised: 3-21-2005

Remarks: Study sponsored by the U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, National Toxicology Program.

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 93%

Remarks: Substance tested is a granular solid

Method

GLP: n/a

Report/Study Year: 1968

Report/Study Number: SDAHT06

Method/Guideline Followed: n/a

Analytical Monitoring:	n/a
Test Type:	28-day oral feed
Species:	Rat
Strain:	n/a
Sex:	Male/female
Route of Administration:	diet
Exposure Period:	28 days
Doses:	1% and 3% of diet
Control Group:	n/a
Frequency of Treatment:	daily
Post Exposure Observation Period:	n/a
Remarks:	range finding study

Results

Value: NOEL >3% of the diet

Remarks: At 3% some slight effects were seen including increased water intake in both sexes and decreased relative weights of liver and kidney in females. In females at the 1% level a decrease was observed in liver weight. Since the effects were only slight and were not accompanied by histological changes in these organs, it was concluded that the test substance did not cause any distinct deleterious effect at feeding levels of up to 3% of diet.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 3. Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name:	5.4_1300-72-7_131
Last Revised:	11-04-2005
Remarks:	n/a

5.6 GENETIC TOXICITY *IN VITRO*

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	65%

Remarks: purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP: yes

Report/Study Year: 1998

Report/Study Number: 98-3380

Method/Guideline Followed: Not indicated; resembles OECD 471

Test Type: *Salmonella* Mutagenicity Test

System: n/a

Test Concentration: Initial and repeat test: 100, 333, 1000, 3333 and 10000 µg active.ingredient / plate

Species/strain: TA1535, TA1537, TA98, TA100.

Metabolic Activation: Rat or hamster liver S9 mix (Aroclor 1254-induced)

Remarks:

Controls: Negative control: vehicle (buffer).
Positive controls: with S9, 2-aminoanthracene; without S9- TA 100 and TA1535, sodium azide; TA98, 4-nitro-o-phenylenediamine, and TA1537, 9-aminoacridine.

Results

Result: Not mutagenic

Cytotoxic Concentration: negative

Results:

	Test result(A)		
Tester strain	Without activation	With activation (rat S9)	With activation (hamster S9)
TA98	-	-	-
TA100	-	-	-
TA1535	-	-	-
TA1537	-	-	-

(A) +/- : positive/negative result; positive controls gave expected responses .

Remarks: Minor remarks The identity of the buffer used is not clear. No information on use of a vehicle was provided

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and

carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA
Print File Name:	5.5_1300-72-7_72
Last Revised:	11-04-2005
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	65%
Remarks:	purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP:	yes
Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	Guideline not indicated. Two independent tests; duplicate cultures/treatment; number of cells 10^6 ; exposure period 4 hours and expression period 2 days; endpoint: forward mutation on TK locus.
Test Type:	Mouse Lymphoma Mutagenicity Test
Test Concentration:	Without S9: 125-2500 µg/mL, based on toxicity; vehicle DMSO (trial 1 and 2) or Fischer's medium (trial 3). With S9: 250-5000 µg/mL, based on toxicity; vehicle Fischer's medium.
Species/strain:	L5178Y mouse lymphoma cells
Metabolic Activation:	S9 mix.
Remarks:	Negative control: vehicle Controls Positive controls: without S9, methylmethane-sulfonate, with S9, methylcholanthrene

Results

Result:	Not mutagenic without metabolic activation, equivocal with metabolic activation
Cytotoxic Concentration:	n/a

Results:

Test no.	Metabolic activation	Doses tested [µg/mL]	Cytotoxicity [% of control survival] at highest dose	Test result(A)
1	Without	125, 250, 500, 1000, 2000, 2500	61	-
	With	250, 500, 1000, 2000, 3000, 4000, 5000	Lethal	+
2	Without	250, 500, 750, 1000, 2000, 2500	58	-
	With	250, 500, 1000, 2000, 3000, 4000	Lethal	-
3	Without	500, 1000, 2000, 3000, 4000, 5000	25	-

(A)+/- : positive/negative result; positive controls gave expected responses

Remarks: n/a

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA

Print File Name: 5.5_1300-72-7_73

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 65%

Remarks: purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP:	Yes
Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	Guideline not indicated; Without S9: two independent tests: 25.5-32.5 hour exposure in presence of Bromodeoxy Uridine (BrdU) with 2 hour incubation without test substance but with BrdU and Colcemid. With S9: one test: 2 hour exposure plus 25.5 hour exposure in presence of BrdU (during the last 2 hours in presence of Colcemid).
Test Type:	Sister Chromatid Exchange Test
System:	n/a
Test Concentration:	500-5000 µg/mL, based on absence of toxicity
Species/strain:	CHO cells
Metabolic Activation:	Rat S9 mix (Aroclor 1254-induced).
Remarks:	Negative control: vehicle Controls Positive controls: without S9, mitomycin-C; with S9, cyclophosphamide.

Results

Result:	Clastogenic without metabolic activation, not clastogenic with metabolic activation.
Cytotoxic Concentration:	n/a
Results:	Cell cycle delay was apparent at concentrations >2513 µg/mL; incubation time was increased.

Test no.	Metabolic activation	Doses tested [µg/mL]	Relative percent SCE treated/SCE control	Test result(A)
1	Without	500, 1667, 5000	10, 12, 35*	+
	With	500, 1667, 5000	4.9, -0.5, 1.2	-
2	Without	2513, 3750, 5000	30*, 40*, 51*	+

(A)+/- : positive/negative result; positive controls gave expected responses.
* Significantly different from controls (linear regression trend versus log dose).

Remarks: n/a

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA
Print File Name:	5.5_1300-72-7_74
Last Revised:	11-04-2005
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	65%
Remarks:	purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP:	yes
Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	Guideline not indicated; Without S9: 18 hour exposure plus 2 hour exposure in presence of Colcemid. With S9: 2 hour exposure plus 10 hour incubation in fresh medium (without test substance, during the last 2 hours in presence of Colcemid).
Test Type:	Chromosome Aberration Test
System:	n/a
Test Concentration:	2513, 3750, 5000 µg/mL, based on absence of toxicity
Species/strain:	CHO cells
Metabolic Activation:	Rat S9 mix (Aroclor 1254-induced)
Remarks:	Controls: Negative control: vehicle. Positive controls: without S9, mitomycin-C; with S9, cyclophosphamide

Results

Result:	Not clastogenic with and without metabolic activation
Cytotoxic Concentration:	n/a

Results:

Test no.	Metabolic activation	Doses tested [µg/mL]	Abberations [%]	Test result(A)
1	Without	2513, 3750, 5000	3.0, 3.5, 3.0	-
	With	2513, 3750, 5000	4.5, 3.0, 3.5	-

(A)+/- : positive/negative result; positive controls gave expected responses .

Remarks: Incubation time was lengthened due to chemical-induced cell cycle delay..

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA

Print File Name: 5.5_1300-72-7_75

Last Revised: 11-04-2005

Remarks: n/a

5.7 GENETIC TOXICITY IN VIVO

Genetic toxicity (in vivo) data were collected for CAS numbers 28088-63-3, and 28348-53-0 (32073-22-6).

5.8 CARCINOGENICITY

Test Substance

CAS Number: 1300-72-7

Identity: Xylene sulfonic acid, sodium salt

Purity: 65%

Remarks: purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP: yes

Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	not indicated; resembles OECD 453
Analytical Monitoring:	At the beginning and every 7-10 weeks thereafter from all concentrations by HPLC
Test Type:	2-year dermal study (with clipped skin)
Species:	Rat, age 6 weeks, mean weight males 127-128g, females 107-108g.
Strain:	F344/N
Sex:	Male/female
No. of animals	50 per sex per dose group
Route of Administration:	dermal
Exposure Period:	2 years
Frequency of Treatment:	5 days/week
Post Exposure Observation Period:	n/a
Doses:	60, 120 and 240 mg active ingredient (a.i.)/kg bw (vehicle 50% ethanol, volume applied 0.1-0.4 mL); volumes adjusted for weight of animals throughout the study; vehicle controls; solutions/suspensions were prepared every 2-3 weeks.
Remarks:	Statistical. method: Kaplan-Meier, logistic regression analysis, life table test, Fisher exact test, Cochran-Armitage trend test Comparison of continuous variables: Dunnett and Williams test, Shirley and Dunn.
	Observations: Twice daily with clinical findings recorded monthly. Body weights recorded weekly through week 13, monthly thereafter. All animals were necropsied with complete histopathological examination on all animals that died prior to study termination, on control rats and on 240 mg/kg bw rats at the end of the study. Skin at sites of application was examined in all animals. Observations were as per OECD 453 with the exception of clinical signs recorded monthly, no food consumption, no blood parameters, no urinalysis and no organ weights.

Results

No evidence of carcinogenic activity

Results:

Dose [mg a.i./kg bw] effect	0		60		120		240		DR	
Sex	M	F	M	F	M	F	M	F	M	F
Mortality	43/50	28/50	33/50	34/50	41/50	33/50	40/50	34/50		

Clinical signs(A)		+				+		+		
Body weight gain	No treatment related effects									
Necropsy	Not reported									
Histopathology										
Epidermal hyperplasia of the application site						+		+		
Lymphnodes ectasia							+			
Seminal vessels atrophy			+		+		+			
Tumours										
Subcutaneous tissue fibroma							+			
Pituitary gland adenoma	+		+		+		+			
Mononuclear leukemia				+				+		
Testes adenoma								+		

(A) Irritation of the skin at the application site.
+ = incidence (biological or statistical significance not indicated)
DR = dose related as indicated by "x"

Remarks:

1. Mononuclear cell leukemia is a common neoplasm in rats of this strain, which is accompanied by enlargement of the lymph nodes. Testicular effects can be attributed to high control values.
2. Incidence and morphology of neoplasms in skin and subcutaneous tissues were consistent with spontaneous neoplasms in F344/N rats and not considered related to treatment.
3. Low incidence of hyperplasia of epidermis at site of application seen in 60, 120 and 240 mg/kg males. Low incidence of hyperplasia at site of application with statistically positive trend seen in control, 120 and 240 mg/kg females. Hyperplasia of epidermis may be related to chemical administration.
4. Hyperplasia of sebaceous glands seen in control and 60 mg/mL males and control, 120 and 240 females.
5. Focal ulceration of epidermis seen in control, 120 and 240 mg/kg females appear related to repeated hair clippings and vehicle application.
6. Lower incidences of pituitary gland adenoma and testicular interstitial cell adenoma in male rats observed not related to treatment.
7. Marginal increases in mononuclear cell leukemia in male rats did not show a clear dose-response relationship and were considered unrelated to treatment.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA
Print File Name:	5.7_1300-72-7_85
Last Revised:	11-04-2005
Remarks:	n/a

Test Substance

CAS Number:	1300-72-7
Identity:	Xylene sulfonic acid, sodium salt
Purity:	65%
Remarks:	purity 65% (11.5% ortho, 38% meta and 15.5% para).

Method

GLP:	yes
Report/Study Year:	1998
Report/Study Number:	98-3380
Method/Guideline Followed:	not indicated; resembles OECD 453
Analytical Monitoring:	At the beginning and every 7-10 weeks thereafter from all concentrations by HPLC
Test Type:	n/a
Species:	Mouse, age 6 weeks, mean weight males 25 g, females 19 g.
Strain:	B6C3F1
Sex:	Male/female
No. of animals	50 per sex per dose group
Route of Administration:	Dermal (to clipped skin)
Exposure Period:	2 years
Frequency of Treatment:	5 days/week
Post Exposure Observation Period:	n/a
Doses:	182, 364 and 727 mg active ingredient (a.i.)/kg bw (vehicle 50% ethanol, volume applied 0.05-0.1 mL); vehicle controls; solutions/suspensions were prepared every 2-3 weeks; feeding *ad libitum*.
Remarks:	Statistical method: Kaplan-Meier, logistic regression analysis, life table test, Fisher exact test, Cochran-Armitage trend test

	Comparison of continuous variables: Dunnett and Williams test, Shirley and Dunn.
Observations	As per OECD 453 with the exception of clinical signs recorded monthly, no food consumption, no blood parameters, no urinalysis and no organ weights.

Results

Result: No evidence of carcinogenic activity

Results: Mean measured concentrations 97-109% of nominal (except in one sample in the mouse study at 364 and 727 mg/kg bw 111-114%); stability in 50% ethanol at room temperature in dark (4 mg/L and 75 mg/L) for 21 and 29 days respectively confirmed.

Dose [mg a.i./kg bw] effect	0		182		364		727		DR	
Sex	M	F	M	F	M	F	M	F	M	F
Mortality	18/50	19/50	13/50	18/50	11/50	18/50	15/50	14/50		
Clinical signs	No treatment related effects									
Body weight gain	No treatment related effects									
Necropsy	Not reported									
Histopathology										
Epidermal hyperplasia of the application site		+			+	+	+	+	x	
Adrenal cortex hyperplasia							+			
Thyroid focular cell hyperplasia							+			
Tumours										
Hepatocellular adenoma								+		
+ = incidence (biological or statistical significance not indicated) DR = dose related as indicated by "x"										

Remarks:

1. In mice incidences of effects (chronic inflammation and hyperplasia of bile ducts epithelium) and neoplasms (hepatocellular adenoma and carcinoma) were increased compared to historical control data for all treatments and controls. This increase was stronger in males than in females. In the livers of males *Heliobacter* bacteria were identified in 6 animals. These bacteria are associated with the observed hepatitis.
2. In female mice the number of hepatocellular adenomas was increased in the high dose group compared with controls and historical data. In absence of a dose response relationship, no toxicological relevance is attributed to this finding.
3. Incidence and morphology of neoplasms in skin and subcutaneous tissues were consistent with spontaneous neoplasms in B6C3F1 mice and not considered related to treatment.
4. Hyperplasia of epidermis at application sites observed in control, 364 and 727 mg/kg males with a statistically positive trend and in females at all doses and control groups. Hyperplasia of epidermis may be related to chemical administration.

5. Incidences of hepatocellular adenoma, carcinoma or combined, hepatitis, and hyperplasia of bile ductular epithelium were generally greater than that expected by spontaneous occurrence. Hepatocellular neoplasm incidences exceeded those of historical controls. Interpretation of treatment-related increases in neoplasms is confounded by evidence of *Helicobacter hepaticus* infections.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 51. U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: National Toxicology Program, Technical Report Series, No. 464, Research Triangle Park, North Carolina, USA

Print File Name: 5.7_1300-72-7_86

Last Revised: 11-04-2005

Remarks: n/a

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Albright & Wilson Ltd. (Marchon Division), Whitehaven, Cumberland, UK. Subchronic (90-day) toxicity study with Halvopon OR in albino rats / R 2822. 1969

Albright & Wilson, Ltd. France IUCLID Data Sheet Sodium Xylenesulphonate. 2000

Chemicals Evaluation and Research Institute (CERI). 1996. Final Report of Bioaccumulation Study of 2,4-dimethyltoluene sulfonic acid, sodium salt. Report Number 51326. Unpublished data

Continental Oil Company. Detergent Hydrotropes/Foam Stabilizers, from Soap and Chemical Specialties. 1965

Continental Oil Company, Ponca City, Oklahoma, USA. Acute oral Toxicity (LD50) in Rats / 202098, 1975a

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Marchon Products Ltd., Whitehaven, Cumberland, UK. Acute oral toxicity of samples A.8969[1] and A.8970[2] in the rat / 1379/65/297. 1965

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA, Static acute toxicity of sodium xylene sulfonate to fathead minnow (*Pimephales promelas*) / 40422, 1992a

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Evaluation for biodegrability in the Modified Sturm Test of Sodium xylenesulfonate [1300-72-7]. 1992c

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA; Acute Toxicity of sodium xylene sulfonate to *Daphnia Magna* / 40424, 1992d

Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® SX / MSDS No. 1-10104. 1997a

SafePharm Laboratories. 2005. Xylene sulfonic acid, sodium salt (93%): Determination of vapour pressure. SPL project number 2098/001

The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Stepan Company, Northfield, Illinois, USA. Stepanate SXS - Toxicity to the freshwater alga, *Selenastrum capricornutum* / 13039.0393.6105.430, 1993a

Stepan Company, Northfield, Illinois, USA; Stepanate SXS ¨C Acute Toxicity to Daphnids (*Daphnia Magna*) under static conditions /13039.0393.6104.110, 1993b

Stepan Company, Northfield, Illinois, USA; Stepanate SXS – Acute Toxicity to Rainbow Trout (*Oncorhynchus mykiss*) under static conditions / 13039.0393.6103.103, 1993c

Stepan Company, Northfield, Illinois, USA. Biotic Degradation (Modified Sturm test) Evaluation, in an aqueous medium, of the "ultimate" biodegradability of substances: 1736-1A, 1736-1B, 1736-1C, 1736-1D, 1736-1E / 16 BF 53. 1993

Tracor Jitco, Inc. Subcontract No. 76-36-106002; GSRI No. 412-798. A repeated dose test of xylene sulfonic acid sodium salt (C55403) in B6C3F1 mice and Fischer 344 rats. July 26, 1979

Tracor Jitco, Inc. Subcontract No. 76-36-106001; GSRI No. 410-798. A subchronic test of xylene sulfonic acid sodium salt (C55403) in B6C3F1 mice and Fischer 344 rats. March 21, 1980

Tracor Jitco, Inc. Subcontract No. 76-36-106002; GSRI No. 410-798. A repeated dose test rerun of xylene sulfonic acid sodium salt (C55403) in Fischer 344 rats. May 19, 1980

U.S. Department of Health and Human Services, Public Health Service, National Institutes of Health, Research Triangle Park, North Carolina, USA. Toxicology and carcinogenesis studies of technical grade sodium xylenesulfonate (CAS No. 1300-72-7) in F344/N Rats and B6C3F1 mice (dermal studies) / NIH No. 98-3380. 1998

Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. >= 1981

Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data

SIDS DOSSIER

CAS NO. 12068-03-0

Toluene sulfonic acid, sodium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
16106-44-8
26447-10-9
28088-63-3
28348-53-0 (32073-22-6)
30346-73-7
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **12068-03-0**

B. Name (IUPAC name) **sodium toluenesulphonate**

C. Name (OECD name) **toluene sulfonic acid, sodium salt**

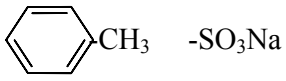
D. CAS Descriptor **Benzenesulfonic acid, methyl-, sodium salt**

E. EINECS-Number **235-088-1**

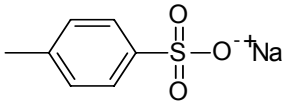
F. Molecular Formula **C7 H7 O3 S1 Na1**

G. Structural Formula

Commercial toluene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the para isomer as a representative structure. An ortho-isomer would have adjacent attachment points to the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.



.



H. Substance Group **Hydrotropes category**

I. Substance Remark

J. Molecular Weight **194 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country: **Australia**

B. Lead Organization:

Name of Lead Organization:

National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
Tel: +61 2 8577 8880

C. Name of responder

Name: Kathleen Stanton, Consortium Manager
Address:
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France

1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six "sponsored" substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of SubstanceError! Bookmark not defined.

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate.

1.2 SYNONYMS

toluene sulfonate, sodium salt
sodium toluene sulfonate
benzenesulfonic acid (1-methyl) sodium salt
methylbenzenesulfonate, sodium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%
Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number: 12068-03-0

Identity: TOLUENESULFONIC ACID, SODIUM SALT

Purity: n/a

Carbon Chain Length Distribution: n/a

Remarks: SMILES: [Na]OS(=O)(=O)c1ccc(cc1)C
MOL FOR: C7 H7 O3 S1 Na1

Method

GLP: n/a

Report/Study Year: n/a

Report/Study Number: EPI-001

Method/Guideline Followed: n/a

Remarks: n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	194.18	
Water Solubility (mg/l):	1e+006	n/a
Octanol Water Partition Coefficient (Log Kow):	-2.40	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	532.98	n/a
Melting Point (°C):	228.00	n/a
Vapor Pressure(mmHg):	2.63E-011	n/a
Henry's Law Constant (atm/(mole/m^3)):	6.720E-018	n/a
Atmospheric Oxidation Half-Life (hours):	105	n/a
Soil Adsorption Coefficient (Log Koc):	1.282	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions

Reference

Source Reference: Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Other References: n/a

Other

Sponsor: n/a
Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.0.1_12068-03-0_162
Last Revised: 11-04-2005
Remarks: n/a

2.1 MELTING POINT

Test Substance

CAS Number: 12068-03-0
Identity: Toluene sulfonic acid, sodium salt
Purity: 94.6%
Remarks: Manufacture: Nacalai Tesque, Inc; Lot No. MOA9562

Method

GLP: no
Report/Study Year: 1996
Report/Study Number: n/a
Method/Guideline Followed: Other: ISO 1218-1975 (E): Plastics – Polyamides – Determination of "melting point"
Analytical Monitoring: n/a
Remarks: n/a

Results

Value: No clear melting point was observed up to 300 degree C
Remarks: n = 2

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions; Full study report is available and is well documented.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 59. Chemicals Evaluation and Research Institute (CERI). 1996. Measurement of Melting Point of o-toluene sulfonic acid, sodium salt. Unpublished data.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a

Print File Name: 2.1_12068-03-0_100
Last Revised: 11-04-2005
Remarks: n/a

2.2 BOILING POINT

Modeled boiling point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Boiling point was measured for CAS numbers 1300-72-7 and 26447-10-9.

2.3 DENSITY

Density was measured for CAS numbers 28088-63-3 and 1300-72-7 (827-21-4).

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW})

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. $\log_{10} K_{ow}$ was measured for CAS number 28088-63-3.

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Test Substance

CAS Number: 12068-03-0
Identity: Toluene sulfonic acid, sodium salt
Purity: > 93%
Remarks: 30-40% aqueous solution

Method

GLP: n/a
Report/Study Year: 1997
Report/Study Number: MSDS No.: 1-10103
Method/Guideline Followed: not indicated
Remarks: n/a

Results

Description: Soluble in water
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference:	45. Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® ST/ MSDS No.: 1-10103. 1997d

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.6.1_12068-03-0_104
Last Revised:	11-04-2005
Remarks:	n/a

3.0.1 EQC MODEL

Fugacity modelling has been conducted on CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	12068-03-0
Identity:	TOLUENESULFONIC ACID, SODIUM SALT
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: [Na]OS(=O)(=O)c1ccc(cc1)C MOL FOR: C7 H7 O3 S1 Na1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 12068030
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	1.22 E-12 cm3/molecule-sec
Half Life	105 hrs

Remarks: n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a

Print File Name:	AOPWOO1 12068030
Last Revised:	05-09-06
Remarks:	n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

REFER SECTION 3.0.1 EQC MODEL.

3.4 BIODEGRADATION

Test Substance

CAS Number:	12068-03-0
Identity:	Toluene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	1965
Report/Study Number:	SDAHT04
Test Type:	aerobic
Method/Guideline Followed:	not indicated
Inoculum:	Two systems, one with natural river microbial flora, the other with raw municipal sewage
Inoculum Acclimated:	no
Control substance:	None

Test Substance Initial Concentration:

Value	Unit	Expressed as
10	mg/L	test substance

Remarks:

- The second system consisted of distilled water containing 5 ppm of yeast extract and was inoculated with 5 mL/liter of raw municipal sewage.
- Analysis: by photospectrometric method (UV). Measured test substance against a blank.

- Temperature: 25 °C.
- Reference substance: None.

Results

Degradation of Toluene sulfonate after 3-days: 100%.

Result:

	1 day	2 days	3 days
Toluene sulfonate	0%	51%	100%

Remarks:

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Not a generally accepted method.

Reference

Source Reference: 6. Continental Oil Company. Detergent Hydrotropes/Foam Stabilizers, from Soap and Chemical Specialties. 1965

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 3.5_12068-03-0_90

Last Revised: 6-29-2004

Remarks: The two biological test systems were found to produce essentially identical results.

Test Substance

CAS Number: 12068-03-0

Identity: Toluene sulfonic acid, sodium salt

Purity: 94.6%

Remarks: Manufacture: Nacalai Tesque, Inc; Lot No. MOA9562

Method

GLP: yes

Report/Study Year: 1996

Report/Study Number: 21323

Test Type: aerobic

Method/Guideline Followed: OECD Guideline 301C “Ready biodegradability: Modified MITI Test (I)”

Inoculum: Activate sludge

Inoculum Acclimated: no

Control substance: Aniline

Test Substance Initial Concentration:

Value	Unit	Expressed as
100	Mg/L	test substance

Remarks: 30 mg of the test substance (n=3) or aniline (n=1) and 9 mg of activated sludge (as MLSS) were added into 300 ml of test medium. Before adding the inoculum, pH values were adjusted to 7 +/- 0.1 by HCl. The test and control vessels were cultivated for 28 days at 25 degree C. Biodegradability continuously measured by a BOD meter. At the end of the test, residual amount of the test substance was determined by TOC and HPLC analysis.

Results

Under test conditions, no biodegradation observed.

Result: Degradation kinetics:

	7 day	14 days	21 days	28 days
Toluene sulfonate	0-1%	0-2%	0-2%	0-2%
Aniline	70%	78%		

Remarks: pH in the test solution at the end of the test was 7.2

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Full study report is available and is well documented.

Reference

Source Reference: 60. Chemicals Evaluation and Research Institute (CERI). 1996. Final Report of Biodegradability Study of o-toluene sulfonic acid, sodium salt. Report Number 21323. Unpublished data.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 3.5_12068-03-0_90

Last Revised: 11-04-2005

Remarks: While a valid test, these results (i.e., “non-biodegradable”) are inconsistent with the results (i.e., “biodegradable”) obtained from the other biodegradation test with toluene sulfonic acid, sodium salt as well from 9 biodegradation tests with the other chemical substances that make up the hydrotropes category.

3.6 BIOACCUMULATION

Test Substance

CAS Number:	12068-03-0
Identity:	Toluene sulfonic acid, sodium salt
Purity:	94.6%
Remarks:	Manufacture: Nacalai Tesque, Inc; Lot No. MOA9562

Method

GLP:	Yes
Report/Study Year:	1996
Report/Study Number:	51323
Method/Guideline Followed:	OECD Guideline 305C: Bioaccumulation, Test for the degree of bioconcentration in Fish.
Species:	*Cyprinus sp.* (freshwater fish)
Exposure Period:	42 days at 25 degree C
Remarks:	A number of fish were exposed to concentrations at 1 and 0.1 µg/L under flow through system. Test concentrations in water and fish were determined by HPLC analysis.

Results

BCF <2.3

Remarks: All measured BCF values were lower than detection limit of HPLC analysis.

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions. Full study report is available and is well documented.
Flag	Critical study for SIDS endpoint

Reference

Source Reference: 61. Chemicals Evaluation and Research Institute (CERI). 1996. Final Report of Bioaccumulation Study of o-toluene sulfonic acid, sodium salt. Report Number 51323. Unpublished data.

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	3.7.1_12068-03-0_104
Last Revised:	11-04-2005
Remarks:	n/a

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Fish toxicity data are available for CAS numbers 1300-72-7(827-21-4), 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2.A ACUTE ORAL TOXICITY

Test Substance

CAS Number: 12068-03-0
Identity: Toluene sulfonic acid, sodium salt
Purity: not indicated
Remarks: 50% aqueous concentration

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Test type: n/a
Species: Rat
Remarks: No details provided

Results

Value: LD50 = 6500 mg/kg
Remarks: 95% confidence interval of 5700 – 7300 mg/kg

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 50 The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 5.1.1_12068-03-0_35
Last Revised: 6-22-2004
Remarks: n/a

5.2.B ACUTE INHALATION TOXICITY

Test Substance

CAS Number: 12068-03-0
Identity: Toluene sulfonic acid, sodium salt
Purity: n/a
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1977
Report/Study Number: SDAHT09
Method/Guideline Followed: CPSC CFR1500.40 of Federal Hazardous Substances Act
Analytical Monitoring: n/a
Test Type: n/a
Species: Albino Rat
Strain: Wistar
Sex: Male/female
Vehicle: n/a
Number of Animals per Dose: 5 per sex
Doses: 557 mg/L
Exposure Period: n/a
Remarks: test substance was powdered form

Results

Value: LC50 >557 mg/L
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 53 Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data.
Other References: 50 The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental Safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File 5.1.2_12068-03-0_121

Name:
Last Revised: 11-04-2005
Remarks: n/a

5.2.C ACUTE DERMAL TOXICITY

Acute Dermal Toxicity data are available for CAS Numbers 28088-63-3 and 28348-53-0.

5.3.A SKIN IRRITATION

Test Substance

CAS Number: 12068-03-0
Identity: Toluene sulfonic acid, sodium salt
Purity: not indicated
Remarks: 50:50 mixture of toluene sulfonic acid, sodium salt and xylene sulfonic acid, sodium salt

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Species: rabbit
Strain: New Zealand albino
Vehicle: n/a
Number of Animals: n/a
Concentration: 40% active solution
Exposure: n/a
Remarks: Applied undiluted to both intact and abraded skin.

Results

Result: Mild to moderate
Primary Dermal Irritation Index (PDII): n/a
Remarks: As defined in the Federal Hazardous Substances Act (FHSA), the product was found not to be a primary irritant.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental Safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	5.2.1_12068-03-0_126
Last Revised:	6-29-2004
Remarks:	n/a

5.3.B EYE IRRITATION

Test Substance

CAS Number:	12068-03-0
Identity:	Toluene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	1978
Report/Study Number:	SDAHT07
Method/Guideline Followed:	n/a
Species:	Rabbit
Strain:	New Zealand albino
Vehicle:	n/a
Number of Animals:	3
Dose:	n/a
Remarks:	20% solution undiluted; not rinsed and rinsed

Results

Result: moderately irritating

Remarks: Non-rinsed showed moderate irritation that was reversed in a few hours. Rinsed showed no irritation.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 5.2.2_12068-03-0_127

Last Revised: 6-22-2004

Remarks: n/a

5.4 SENSITIZATION

Test Substance

CAS Number: 12068-03-0

Identity: Toluene sulfonic acid, sodium salt

Purity: n/a

Remarks: n/a

Method

GLP: Yes

Report/Study Year: 1995

Report/Study Number: HS-95/0146

Method/Guideline Followed: OECD 406

Analytical Monitoring: n/a

Test Type: Buehler test

Vehicle: deionized water

Number of Animals: 33

Species: Guinea pig (Dunkin Hartley, Pirbright White)

Concentration:

Type	Value	Unit	Application Form
Induction I, II, III	42.8	%	dermal, semiocclusive
Challenge	42.8	%	dermal, semiocclusive

Remarks: n/a

Results

Result: not sensitizing

Classification: not sensitizing

Remarks: 0/20 animals

Data Quality

Reliability (Klimisch): 1

Remarks: Guideline study

Reference

Source Reference: Hüels AG. Prüfung auf Sensibilisierung der Haut von Na-Toluolsulfonat am Meerschweinchen (Methode nach Bühler), 1995b

Other References:	n/a

Other

Sponsor:	Hüels AG
Submitting Agency:	Hydrotrope Consortium, K.Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	Hüls AG, Prüfinstitut für Toxikologie
Print File Name:	
Last Revised:	6-28-2005
Remarks:	

5.5 REPEATED DOSE TOXICITY

Repeated dose toxicities were measured for CAS numbers 1300-72-7 (827-21-4) and 28348-53-0 (32073-22-6).

5.6 GENETIC TOXICITY *IN VITROERROR! BOOKMARK NOT DEFINED.*

Genetic toxicity (*in vitro*) data were collected for CAS numbers 1300-72-7 (827-21-4) and 28088-63-3, and 28348-53-0 (32073-22-6).

5.7 GENETIC TOXICITY IN VIVO

Genetic toxicity (in vivo) data were collected for CAS numbers 28088-63-3, and 28348-53-0 (32073-22-6).

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Chemicals Evaluation and Research Institute (CERI). 1996. Final Report of Bioaccumulation Study of o-toluene sulfonic acid, sodium salt. Report Number 51323. Unpublished data

Continental Oil Company. Detergent Hydrotropes/Foam Stabilizers, from Soap and Chemical Specialties. 1965

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Hüels AG. Prüfung auf Sensibilisierung der Haut von Na-Toluolsulfonat am Meerschweinchen (Methode nach Bühler), 1995b

Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® ST/ MSDS No.: 1-10103. 1997d

The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 – 1978

Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data

SIDS DOSSIER

CAS NO. 26447-10-9

Xylene sulfonic acid, ammonium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
12068-03-0
16106-44-8
28088-63-3
28348-53-0 (32073-22-6)
30346-73-7
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1. GENERAL INFORMATION

1.01 SUBSTANCE INFORMATION

A. CAS number **26447-10-9**

B. Name *(IUPAC name)* **ammonium xylenesulfonate**

C. Name *(OECD name)* **xylene sulfonic acid, ammonium salt**

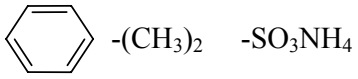
D. CAS Descriptor **Benzenesulfonic acid, dimethyl-, ammonium salt**

E. EINECS-Number **247-710-9**

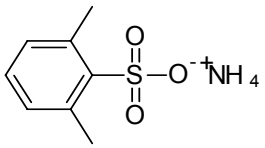
F. Molecular Formula **C8 H13 N1 O3 S1**

G. Structural Formula

Commercial xylene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the ortho, ortho isomer as a representative structure. A para-isomer would have attachments at opposite ends of the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.



.



H. Substance Group **Hydrotropes category**

I. Substance Remark

J. Molecular Weight **203 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country: Australia

B. Lead Organization:

Name of Lead Organization:
National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
Tel: +61 2 8577 8880

C. Name of responder

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France

1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six "sponsored" substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate or

1.2 SYNONYMS

xylenesulfonic acid, ammonium salt
xylenesulfonate, ammonium salt
ammonium xylene sulfonate
benzenesulfonic acid (1-dimethyl) ammonium salt
dimethylbenzenesulfonate, ammonium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%

Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number:	26447-10-9
Identity:	Xylene sulfonic acid, ammonium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: Cc1cc(S(=O)(=O)ON(H)(H)(H)H)cc(C)c1 MOL FOR: C8 H13 N1 O3 S1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	EPI-001
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	203.26	
Water Solubility (mg/l):	5.409e+004	n/a
Octanol Water Partition Coefficient (Log Kow):	-0.13	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	467.92	n/a
Melting Point (°C):	197.61	n/a
Vapor Pressure(mmHg):	2.67E-009	n/a
Henry's Law Constant (atm/(mole/m^3)):	1.320E-014	n/a
Atmospheric Oxidation Half-Life (hours):	41	n/a
Soil Adsorption Coefficient (Log Koc):	2.889	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions.

Reference

Source Reference: Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Other References: n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.0.1_26447-10-9_164
Last Revised:	11-4-2005
Remarks:	n/a

2.1 MELTING POINT

Modeled melting point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Melting point was measured for CAS numbers 12068-03-0, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

2.2 BOILING POINT

Test Substance

CAS Number:	26447-10-9
Identity:	Xylene sulfonic acid, ammonium salt
Purity:	Not indicated
Remarks:	40% aqueous solution

Method

GLP:	n/a
Report/Study Year:	1997
Report/Study Number:	MSDS No.: 1-10105
Method/Guideline Followed:	not indicated
Analytical Monitoring:	n/a
Remarks:	n/a

Results

Value: 101 ˚C

Remarks: Result reflects boiling point of aqueous solution and therefore of water. The chemical substance is an ionic solid. Hydrotropes are produced as either aqueous solutions or as granular solids.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 43 Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® 4AX / MSDS No.: 1-10105. 1997b

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.2_26447-10-9_102
Last Revised:	11-04-2005
Remarks:	n/a

2.3 DENSITY

Density was measured for CAS numbers 28088-63-3 and 1300-72-7 (827-21-4).

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW})

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. log_{10} K_{ow} was measured for CAS number 28088-63-3.

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Test Substance

CAS Number:	26447-10-9
Identity:	Xylene sulfonic acid, ammonium salt
Purity:	40%
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	1997
Report/Study Number:	MSDS No.: 1-10105
Method/Guideline Followed:	not indicated
Remarks:	n/a

Results

Description: Completely soluble in water

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 43. Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® 4AX / MSDS No.: 1-10105. 1997b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 2.6.1_26447-10-9_103

Last Revised: 11-04-2005

Remarks: n/a

3.0.1 EQC MODEL

Fugacity modelling has been conducted on CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	26447-10-9
Identity:	Xylene sulfonic acid, ammonium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: Cc1cc(S(=O)(=O)ON(H)(H)(H)H)cc(C)c1 MOL FOR: C8 H13 N1 O3 S1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 26447109
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	3.11 E-12 cm3/molecule-sec
Half Life	41 hrs
Remarks:	n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File	AOPWOO1 26447109

Name:
Last Revised: 05-09-06
Remarks: n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

REFER SECTION 3.0.1 EQC MODEL.

3.4 BIODEGRADATION

Test Substance

CAS Number: 26447-10-9
Identity: Xylene sulfonic acid, ammonium salt
Purity: n/a
Remarks: n/a

Method

GLP: n/a
Report/Study Year: n/a
Report/Study Number: SDAHT02
Test Type: aerobic
Method/Guideline Followed: not indicated
Inoculum: not indicated
Inoculum Acclimated: n/a

Test Substance Initial Concentration:

Value	Unit	Expressed as
20	mg/L	Test substance

Remarks: CO_2 evolution during screening assays for ultimate biodegradability. Test compound used as sole carbon source. Test duration was 26 days.

Results

Kinetics Measured as: CO_2
Remarks: Biodegradation 71% $THCO_2$, 26 days, 2-day lag period observed.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference:	17. Procter & Gamble Company, Environmental Safety Assessment for Xylene Sulfonate, post 1981.
Additional Reference	50. The Soap and Detergent Association, Washington, DC USA. Summary of Human and Environmental Data on Hydrotropes. SDAHT07. 1973-1978

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	3.5_26447-10-9_89
Last Revised:	5-20-2005
Remarks:	n/a

3.6 BIOACCUMULATION

Estimated data is available for this CAS number in EPISuite estimation of Physical/Chemical Properties in 2.0.1. Measured data is available for CAS numbers 12068-03-0 and 1300-72-7 (827-21-4).

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number: 26447-10-9

Identity: Xylene sulfonic acid, ammonium salt

Purity: not indicated

Remarks: n/a

Method

GLP: n/a

Report/Study Year: post-1981 ??

Report/Study Number: SDAHT02

Method/Guideline Followed: not indicated

Test Type: n/a

Analytical Monitoring: n/a

Species: bluegill

Exposure Period:

Value	Unit
96	hour(s)

Remarks: n/a

Results

Unit: mg/L

Results: 96-hr LC50 = 1060 mg/L

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature

Reference

Source Reference: 17 Procter & Gamble Company, Environmental Safety Assessment for Xylene Sulfonate, ≥ 1981.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.1_26447-10-9_7

Last Revised: 6-21-2004

Remarks: n/a

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2.A ACUTE ORAL TOXICITY

Test Substance

CAS Number: 26447-10-9
Identity: Xylene sulfonic acid, ammonium salt
Purity: Not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1981
Report/Study Number: SDAHT03
Method/Guideline Followed: not indicated
Test type: n/a
Species: Rat
Remarks: No details provided

Results

Value: Oral LD50 > 2100 mg/kg
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 52 Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. ≥ 1981

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: Some data appear to be from Conoco and some from Unilever (can this be more specific; it's confusing)
Print File Name: 5.1.1_26447-10-9_33
Last Revised: 6-22-2004
Remarks: n/a

5.2.B ACUTE INHALATION TOXICITY

Test Substance

CAS Number: 26447-10-9
Identity: Xylene sulfonic acid, ammonium salt
Purity: not indicated

Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1981
Report/Study Number: SDAHT03
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Test Type: n/a
Species: Rabbit
Strain: n/a
Sex: n/a
Vehicle: n/a
Number of Animals per Dose: n/a
Doses: 6.41 mg/L

Exposure Period:

Value	Unit
4	hours

Remarks: air flow equal 24 liters per minute

Results

Value: LC50 > 6.41 mg/L
Remarks: 100% survival

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 52 Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. ≥ 1981

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 5.1.2_26447-10-9_124
Last Revised: 6-22-2004
Remarks: cited as Conoco

5.2.C ACUTE DERMAL TOXICITY

Acute dermal toxicity data are available for CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

5.3.A SKIN IRRITATION

Test Substance

CAS Number: 26447-10-9
Identity: Xylene sulfonic acid, ammonium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1981
Report/Study Number: SDAHT03
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Species: Rabbit
Vehicle: n/a
Number of Animals: n/a
Concentration: 40% solution
Exposure: n/a
Remarks: n/a

Results

Result: slightly irritating
Primary Dermal Irritation Index (PDII): n/a
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 52. Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. ≥ 1981

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: Overview of available data
Print File Name: 5.2.1_26447-10-9_56
Last Revised: 6-22-2004
Remarks: n/a

5.3.B EYE IRRITATION

Test Substance

CAS Number: 26447-10-9

Identity: Xylene sulfonic acid, ammonium salt

Purity: Not indicated

Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1981

Report/Study Number: SDAHT03

Method/Guideline Followed: not indicated

Species: Rabbit

Vehicle: n/a

Number of Animals: n/a

Dose: n/a

Remarks: n/a

Results

Result: slightly irritating

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 52. Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate. ≥ 1981

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Overview of available data

Print File Name: 5.2.2_26447-10-9_57

Last Revised: 6-22-2004

Remarks: Some data are from Conoco and some from Unilever

5.4 SENSITIZATION

Skin sensitization data are available for CAS numbers 12068-03-0, and 28348-53-0 (32073-22-6).

5.5 REPEATED DOSE TOXICITY

Repeated dose toxicities were measured for CAS numbers 1300-72-7 (827-21-4) and 28348-53-0 (32073-22-6).

5.6 GENETIC TOXICITY *IN VITRO*

Genetic toxicity (*in vitro*) data were collected for CAS numbers 1300-72-7 (827-21-4) and 28088-63-3, and 28348-53-0 (32073-22-6).

5.7 GENETIC TOXICITY IN VIVO

Genetic toxicity (in vivo) data were collected for CAS numbers 28088-63-3, and 28348-53-0 (32073-22-6).

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Procter & Gamble Company, Environmental Safety Assessment for Xylene Sulfonate ≥ 1981

Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® 4AX / MSDS No.: 1-10105. 1997b

The Soap and Detergent Association, Washington, DC USA. Summary of Human and Environmental Data on Hydrotropes. SDAHT07. 1973-1978

Unilever Research Laboratory. Human Safety Perspective for Xylene Sulfonate ≥ 1981

SIDS DOSSIER

CAS NOs. 28348-53-0 (32073-22-6)

Cumenesulfonic acid, sodium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
12068-03-0
16106-44-8
26447-10-9
28088-63-3
30346-73-7
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **28348-53-0**

(also 32073-22-6)

B. Name *(IUPAC name)* **sodium cumenesulphonate**

(cumene, monosulpho derivative, sodium salt)

C. Name *(OECD name)* **cumene sulfonic acid, sodium salt**

(same)

D. CAS Descriptor **Benzenesulfonic acid, (1-methylethyl)-, sodium salt**

(Benzene, (1-methylethyl)-, monosulfo derive., sodium salt)

E. EINECS-Number **248-983-7**

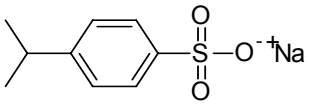
(250-913-5)

F. Molecular Formula **C9 H11 O3 S1 Na1**

G. Structural Formula

Commercial cumene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the para isomer as a representative structure. An ortho-isomer would have adjacent attachment points on the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.

.



H. Substance Group **Hydrotropes category**

I. Substance Remark **The same substance is identified by two CAS numbers**

J. Molecular Weight **222 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country: Australia

B. Lead Organization:

Name of Lead Organization:
National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
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C. Name of responder

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1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six "sponsored" substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate or

1.2 SYNONYMS

cumenesulfonic acid, sodium salt
cumenesulfonate, sodium salt
sodium cumene sulfonate
benzenesulfonic acid (1-methylethyl) sodium salt
methylethylbenzenesulfonate, sodium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:
Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%
Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: n/a

Carbon Chain Length Distribution: n/a

Remarks: SMILES: [Na]OS(=O)(=O)c1ccc(cc1)C(C)C
MOL FOR: C9 H11 O3 S1 Na1

Method

GLP: n/a

Report/Study Year: n/a

Report/Study Number: EPI-001

Method/Guideline Followed: n/a

Remarks: n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	222.24	
Water Solubility (mg/l):	6.346e+005	n/a
Octanol Water Partition Coefficient (Log Kow):	-1.50	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	549.19	n/a
Melting Point (°C):	235.58	n/a
Vapor Pressure(mmHg):	8.19E-012	n/a
Henry's Law Constant (atm/(mole/m^3)):	3.774E-018	n/a
Atmospheric Oxidation Half-Life (hours):	39.5	n/a
Soil Adsorption Coefficient (Log Koc):	1.766	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions

Reference

Source Reference: Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Other References: n/a

Other

Sponsor: n/a
Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.0.1_28348-53-0_165
Last Revised: 11-04-2005
Remarks: n/a

2.1 MELTING POINT

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: 88-93%.
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1997
Report/Study Number: MSDS Ref No.: PSMSD-287
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Remarks: n/a

Results

Value: 182.2 °C
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 1 Albright & Wilson Americas Inc., Glen Allen, Virginia, USA. Material Safety Data Sheet Eltesol SC 93 / MSDS Ref No.: PSMSD-287. 1997

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.1_28348-53-0_106

Last Revised: 6-19-2004
Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: >93%
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1997
Report/Study Number: MSDS No. 1-10100
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Remarks: n/a

Results

Value: 300 ˚C
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 44 Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® SC / MSDS No. 1-10100. 1997c

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.1_28348-53-0_108
Last Revised: 6-19-2004
Remarks: n/a

2.2 BOILING POINT

Modeled boiling point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Boiling point was measured for CAS numbers 1300-72-7 and 26447-10-9.

2.3 DENSITY

Density was measured for CAS numbers 28088-63-3 and 1300-72-7 (827-21-4).

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW})

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. log_{10} K_{ow} was measured for CAS number 28088-63-3.

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	1995
Report/Study Number:	SDAHT05
Method/Guideline Followed:	not indicated
Remarks:	in water

Results

Value: 400 g/L at 20 °C

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 10. Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate. 1995

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.6.1_28348-53-0_105

Last Revised: 11-04-2005
Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: 88-93%
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1997
Report/Study Number: MSDS Ref No.: PSMSD-287
Method/Guideline Followed: not indicated
Remarks: n/a

Results

Value: Water Solubility: 33g/100g H_2O ; equivalent to 330g/L
Remarks:

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 1. Albright & Wilson Americas Inc., Glen Allen, Virginia, USA. Material Safety Data Sheet Eltesol SC 93 / MSDS Ref No.: PSMSD-287. 1997

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 2.6.1_28348-53-0_107
Last Revised: 6-19-2004
Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: >93%
Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1997

Report/Study Number: MSDS No. 1-10100

Method/Guideline Followed: not indicated

Remarks: n/a

Results

Description: Soluble in water

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 44. Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® SC / MSDS No. 1-10100. 1997c

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 2.6.1_28348-53-0_109

Last Revised: 11-04-2005

Remarks: n/a

3.0.1 EQC MODEL

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	"pure"
Remarks:	n/a

Method

Report/Study Year:	2003
Report/Study Number:	SDAHT10
Method/Guideline Followed:	Fugacity Level III; version 2.02
Test Type:	modelling
Media:	n/a
Remarks:	Input parameters were based on measured or EPIWIN-modelled physico-chemical properties of the test material. Water solubility = 330,000 mg/L; octanol water partition coefficient = -1.5; melting point = 300 ^{o}C; vapor pressure = 1.09 x 10^{-9}. Total mass used as release volume = 3310.5 kg/h to water (based on 29,000 tonnes released over 356 days, 24 hours per day). Emission levels used for Level II modeling would be the default 1000 kg/h to water, air, sediment.

Results

Level III

Air (%)	Water (%)	Soil (%)	Sediment (%)
0	99.9	0.1	0

Remarks: The outputs for both Level II and III are almost identical.

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions. Modelling estimate based on some measured and some estimated input parameters.

Reference

Source Reference:	Trent University Canadian Environmental Modeling Centre at www.trentu.ca/cemc/welcome.html.
Other References:	Mackay D., A. DiGuardo, S. Paterson and C. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environmental Toxicology and Chemistry (15) 9: 1627-1637.

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name:	3.3.1_28348-53-0_119

Last Revised: 11-04-2005
Remarks: n/a

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: [Na]OS(=O)(=O)c1ccc(cc1)C(C)C MOL FOR: C9 H11 O3 S1 Na1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 28348530
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	3.26 E-12 cm3/molecule-sec
Half Life	39 hrs

Remarks: n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File	AOPWOO1 28348530

Name:
Last Revised: 05-09-06
Remarks: n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

REFER SECTION 3.0.1 EQC MODEL.

3.4 BIODEGRADATION

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	45%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	yes
Report/Study Year:	1993
Report/Study Number:	40427
Test Type:	aerobic
Method/Guideline Followed:	OECD 301B. Modified Sturm Test
Inoculum:	activated sludge
Inoculum Acclimated:	yes
Acclimated to what Concentration:	20 mg C/L
Acclimated for what Duration:	19 days
Control Substance:	sodium acetate

Test Substance Initial Concentration:

Value	Unit	Expressed as
10	mg/L	OrganicCarbon (OC)
20	mg/L	OC

Control Substance

Value	Unit	Expressed as

Initial Concentration:	20	mg/L	OC

Remarks:

- Pre-acclimation phase: 9 days, thereafter SCAS test.
- Amount: approximately 500 mL was used for the SCAS test.
- Temperature: 22 ± 3 °C.
- Analysis: CO_2 produced was trapped in the KOH solutions in the gas-washing bottles.
- Analysis on day 2, 4, 6, 8, 10, 15, 20, 25 and 28.

Results

Results: results in %$THCO_2$

day	2	4	6	8	10	15	20	25	28
10 mg Carbon/L	4.96	34.66	65.31	89.38	96.24	102.44	106.36	106.36	109.43
20 mg C/L	2.75	13.18	82.03	86.75	88.54	96.69	100.46	100.46	103.21
Reference	17.85	29.00	80.81	83.15	85.30	92.62	93.21	93.21	93.21

The substance is biodegradable (> 60% $THCO_2$ within 28 days), more than 60% after 6 days.

Remarks: n/a

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 26. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Aerobic biodegradation of sodium cumenesulfonate in the modified Sturm test / 40427. 1993

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 3.5_28348-53-0_92

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1994

Report/Study Number: SDAHT01

Test Type: aerobic

Remarks: Coupled unit test; OECD Screen Test; Zahn Wellens Test

Results

Result: readily biodegradable

Remarks:

Guideline	*Biodegradation*
Coupled Unit	82.5-91.5%
OECD 301 E, screening	94%
OECD 302B, Zahn Wellens	100%

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature. Publication lacks study detail.

Reference

Source Reference: 7. Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 3.5_28348-53-0_94

Last Revised: 6-29-2004

Remarks: n/a

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: 88-93%

Remarks: Substance tested is a granular solid

Method

GLP: n/a

Report/Study Year: 1978
Report/Study Number: SDAHT07
Test Type: aerobic
Method/Guideline Followed: not indicated
Remarks: n/a

Results

Remarks: Biodegradation 73% CO_2 in standard test

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978
Other References: Standard CO2 Test – Journal American Oil Chem. Soc. Vol 50, May 1973.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 3.5_28348-53-0_96
Last Revised: 6-29-2004
Remarks: n/a

3.6 BIOACCUMULATION

Estimated data is available for this CAS number in EPISuite estimation of Physical/Chemical Properties in 2.0.1. Measured data is available for CAS numbers 12068-03-0 and 1300-72-7 (827-21-4).

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	45%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	yes
Report/Study Year:	1992
Report/Study Number:	40421
Method/Guideline Followed:	EPA-TSCA 797.1400.
Test Type:	acute, static
Analytical Monitoring:	no
Species:	*Pimephales promelas*, mean length 23 ± 2 mm

Exposure Period:

Value	Unit
96	hour(s)

Remarks: Statistical method: Binominal, moving average and probit analysis.
Number of fish: 10/test vessel, 2 test vessels/treatment.
Concentrations: Nominal: 100, 180, 320, 560 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Test conditions: Static without aeration; at 22 ± 1 °C in 19 L glass vessels containing 15 L of medium of hardness 140 mg/L (as $CaCO_3$) and pH 8.2; 16 hours light; unfed.
Phys. meas.: At 0, 48 and 96 hours: overall ranges for pH 8.0-8.3; O_2 >60%; temperature 22-23 °C.
Observations: Mortality/symptoms at 24, 48, 72 and 96 hours.
Minor remark. Fish were not fed for 72 hours prior to test initiation rather than 24 hours as stated in OECD 203

Results

Unit: mg/L

Remarks:

		Nominal Concentration (mg/L)					
Parameter	Time [hour]	0	100	180	320	560	1000
Mortality [%]	96	None					
Symptoms*	0-96						+

* Symptoms including surfacing and quiescence observed as indicated (+).

96-hr LC50 > 1000 mg/L (equivalent to >450 mg/L active ingredient taking into account the 45% purity of the sample).

NOEC = 560 mg/L

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. No analyses

Flag Critical study for SIDS endpoint

Reference

Source Reference: 41 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA; Statis acute toxicity of sodium cumene sulfonate to fathead minnow (Pimephales promelas) / 40421. 1992e

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 4.1_37475-88-0_5

Last Revised: 11-04-2005

Remarks: n/a. .

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: no

Report/Study Year: n/a

Report/Study Number: SDAHT05

Method/Guideline Followed: Bestimmung der Wirkung von Wasserinhaltsstoffen auf Fische, DIN 38412 Teil 15

Test Type: static

Analytical Monitoring: no

Species: *Leuciscus idus*

Exposure Period:

Value	Unit
48	hour(s)

Remarks: n/a

Results

Unit: mg/L

Results: 48-hr LC50 > 1000 mg/L

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature

Reference

Source Reference: 10 1995 Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.1_28348-53-0_8

Last Revised: 6-21-2004

Remarks: Most likely the same data as for bibliographic reference Chemosphere, Vol 28, No. 12, pp 2203-2236

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: n/a

Report/Study Year: 1994

Report/Study Number: SDAHT01

Method/Guideline Followed: not indicated

Test Type: n/a

Analytical Monitoring: n/a

Species: n/a

Exposure Period:

Value	Unit
48	hour(s)

Remarks: n/a

Results

Unit: mg/L

Results: 48-hr LC50 > 1000 mg/L

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 7 Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.1_28348-53-0_10

Last Revised: 6-21-2004

Remarks: Most likely the same data as reported in source reference Huels AG. IUCLID Data Sheet. 1995.

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: no

Report/Study Year: 1987

Report/Study Number: SDAHT05

Method/Guideline Followed: Verlaengerter Toxizitaetstest bei Daphnia magna nach UBA (1984)

Test Type: reproduction

Analytical Monitoring: no

Species: Daphnia

Exposure Period:

Value	Unit
21	day(s)

Remarks: Report indicates testing was done in 1987 without formal GLP but that GLP certification of the laboratory was received in 1989/1990. Test substance concentrations were 30, 100 and 300 mg/L as active ingredient.

Results

Results: 21-day EC50 reported as 154 mg/L
NOEC reported as <30 mg/L

Remarks: There was no significant test substance related mortality of parent animals. The average number of offspring produced per day was 43 in the controls, 38 at 30 mg/L, 29 at 100 mg/L and 13 at 300 mg/L which equates to 88%, 67% and 30% of control response, respectively. It is uncertain whether 88% at 30 mg/L is a significant reduction but the report cites a NOEC of <30 mg/L. No statistical analysis is reported.
The published account of this same study appears in Chemosphere Volume 28, Number 12, pages 2203-2236 (Greim et. Al.); in that published account the NOEC is reported as > 30 mg/L.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary Literature

Flag Critical study for SIDS endpoint

Reference

Source Reference: 10 1995 Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.2_28348-53-0_26

Last Revised: 11-04-2005

Remarks: Based on the conflicting reports, it is uncertain whether the 21-day NOEC is > or < 30 mg/L.

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	not indicated
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	SDAHT01
Method/Guideline Followed:	n/a
Test Type:	n/a
Analytical Monitoring:	n/a
Limit Test:	n/a
Species:	Daphnia
Exposure Period:	Value Unit

21	day(s)

Remarks: n/a

Results

Results: 21-day EC50 reported as 154 mg/L
NOEC reported as >30 mg/L

Remarks: No details are provided except the results.
This same study is cited in Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate, 1995, but the result reported therein indicate NOEC < 30 mg/L.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Publication lacks study details.

Reference

Source Reference: 7 Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.2_28348-53-0_28

Last Revised: 6-21-2004

Remarks: Based on the conflicting reports, it is uncertain whether the 21-day NOEC is > or < 30 mg/L.

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	45%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	yes
Report/Study Year:	1992
Report/Study Number:	40423
Method/Guideline Followed:	EPA-TSCA 797-1300
Test Type:	acute, static
Analytical Monitoring:	no

Species: *Daphnia magna*, <24 hours old

Exposure Period:

Value	Unit
48	hour(s)

Remarks: Number of daphnids: 10/beaker, 2 beakers/treatment.
Concentrations: Nominal: 100, 180, 320, 560 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Test conditions: Static without aeration; at 20 ± 2 °C in 250 mL glass vessels containing 200 mL of medium of hardness 146 mg/L ($CaCO_3$) and pH 8.2; 16 hours light, unfed.
Physical measurements: At 0 and 48 hours: overall ranges for pH 8.2-8.4; O_2 86-89%; temperature 20-21 °C.
Observations: Immobility/symptoms at 24 and 48 hours.

Results

Unit: mg/L

Results:

		Nominal Concentration (mg/L)					
Parameter	Time [hours]	0	100	180	320	560	1000
Immobility [%]	48	0	0	0	0	5	0
Symptoms	48	No treatment related effects					

48-h EC50 >1000 mg/L (equivalent to 450 mg/L active ingredient considering the 45% sample purity).

Remarks:

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. No analyses

Flag Critical study for SIDS endpoint

Reference

Source Reference: 19 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA, Acute toxicity of sodium cumene sulfonate to *Daphnia magna* / 40423. 1992b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: INERIS, Verneuil-en-Halatte, France

Print File Name: 4.2_28348-53-0_16

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: no
Report/Study Year: n/a
Report/Study Number: SDAHT05
Method/Guideline Followed: DIN 38412 Teil 11, Daphnien-Kurzzeittest, Bestimmung der Wirkungvon Wasserinhaltsstoffen auf Kleinkrebse
Test Type: growth rate
Analytical Monitoring: no
Species: *Daphnia magna*

Exposure Period:

Value	Unit
24	hour(s)

Remarks: n/a

Results

Results: 24-hour EC50 > 1000 mg/L
Remarks: No details reported.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary Literature

Reference

Source Reference: 10 1995 Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 4.2_28348-53-0_17
Last Revised: 6-21-2004
Remarks: n/a

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: not indicated

Remarks: n/a

Method

GLP: no

Report/Study Year: 1987

Report/Study Number: SDAHT05

Method/Guideline Followed: Algenwachstumus-Hemmtest nach UBA (1984)

Analytical Monitoring: no

Species: *Scenedesmus subspicatus*

Endpoint: Growth rate

Exposure Period:

Value	Unit
72	Hour(s)

Remarks: n/a

Results

Results: 72-hour EC50 >1000 mg/L

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature

Flag Critical study for SIDS endpoint

Reference

Source Reference: 10 1995 Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 4.3_28348-53-0_23

Last Revised: 11-04-2005

Remarks: n/a

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: no

Report/Study Year: n/a
Report/Study Number: SDAHT05
Test type: aquatic
Method/Guideline Followed: Bringmann-Kuehn-Test
Analytical Monitoring: no
Species: *Pseudomonas putida*

Exposure Period:

Value	Unit
48	hour(s)

Remarks: n/a

Results

Results: 48-hour EC50 >16,000 mg/L
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature
Flag Critical study for SIDS endpoint

Reference

Source Reference: 10 1995 Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 4.4_28348-53-0_25
Last Revised: 11-04-2005
Remarks: n/a

5.2.A ACUTE ORAL TOXICITY

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: 96.0%
Remarks: Substance tested is a granular solid

Method

GLP: no
Report/Study Year: 1982
Report/Study Number: 0019
Method/Guideline Followed: OECD 401
Test type: n/a
Species: Rat
Number of Animals per Dose: 5/sex/dose group
Doses: Single oral administration of 7000 mg/kg bw (vehicle water); no controls; feeding *ad libitum* (food was withheld 16 hours prior to dosing).
Remarks: Observations:

- Mortality/clinical signs continuously for 6 hours on day 1 and daily until day 14.
- Body weights on day 1, 7 and 14.
- Necropsy on day 14 (3/sex/dose group).

Results

Value: Oral LD50 >7000 mg/kg bw

Remarks:

Dose [mg/kg bw] effect		7000		DR	
Sex	Day	M	F	M	F
Mortality	1-14	0/5	2/5		
Clinical signs(A)	1-14	+	+		
Body weight	1-14	No treatment related effects			
Necropsy(B)	14		+		

(A)Clinical observations included increased piloerection, ataxia, lateral recumbency and increased water intake (lasting 24 hours after dosing).
(B)In the animals that died redness of the stomach mucosa was observed.
DR is dose related. (delete this column and line; it's not dose related since there was only one dose.)

No individual data were presented. The report was limited to the above mentioned.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Non GLP. Limited study detail.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 11 Huels AG, Marl, Germany. Akute orale Toxizität von Na-Cumolsulfonat / 0019. 1982a

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: n/a

Print File Name: 5.1.1_28348-53-0_36

Last Revised: 11-04-2005

Remarks: Most likely the same results as reported in Huels IUCLID data sheet 1995 and in Chemosphere Vol 28, No 12, pp 2203-2236.

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: no

Report/Study Year: 1981

Report/Study Number: SDAHT05

Method/Guideline Followed: OECD Guideline 401

Test type: n/a

Species: Rat

Remarks: No details provided

Results

Value: Oral LD50 >7000 mg/kg

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature

Reference

Source Reference: 10 Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate. 1995

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 5.1.1_28348-53-0_37

Last Revised: 6-22-2004

Remarks: Most likely same result as reported in Chemosphere Vol 28, No 12, pp 2203-2236 and in Huels AG 1982 report "Akute orale Toxizitat von Na-Cumolsulfonat / 0019.

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: n/a

Report/Study Year: n/a

Report/Study Number: SDAHT01

Method/Guideline Followed: not indicated

Test type: n/a

Species: Rat

Remarks: No details provided

Results

Value: Oral LD50 >7000 mg/kg

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Publication lacks study details.

Reference

Source Reference: 7 Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 5.1.1_28348-53-0_38

Last Revised: 6-22-2004

Remarks: Most likely the same results as reported in Huels AG IUCLID data sheet 1995 and in 1982 Huels AG report "Akute orale Toxizitat von Na-Cumolsulfonat / 0019.

5.2.B ACUTE INHALATION TOXICITY

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: n/a
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1977
Report/Study Number: SDAHT09
Method/Guideline Followed: CPSC CFR1500.40 of the Federal Hazardous Substances Act
Analytical Monitoring: n/a
Test Type: n/a
Species: Albino Rat
Strain: Wistar
Sex: Male/female
Vehicle: n/a
Number of Animals per Dose: 10 (5 males, 5 females)
Doses: 770 mg/L
Exposure Period: n/a
Remarks: powdered test substance

Results

Value: LC50 > 770 mg/L
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 53 Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data.
Other References: 50 The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental Safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: n/a
Print File Name: 5.1.2_28348-53-0_123

Last Revised: 11-04-2005
Remarks: n/a

5.2.C ACUTE DERMAL TOXICITY

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Test Type: n/a
Species: Rabbit
Remarks: No details provided

Results

Value: Dermal LD50 >2000 mg/kg
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 50 The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.1.3_28348-53-0_44
Last Revised: 6-22-2004
Remarks: n/a

5.3.A SKIN IRRITATION

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: 96.0%
Remarks: 60% aqueous solution

Method

GLP: No
Report/Study Year: 1982
Report/Study Number: 0020
Method/Guideline Followed: OECD 404.
Analytical Monitoring: n/a
Species: Rabbit; weight 2.2-2.4 kg.
Strain: Small White Russian
Vehicle: Aqua dist.
Number of Animals: 3 males and 3 females
Concentration: 60% in aqua dist. (paste)
Exposure: Application of 0.5 mg test substance (no vehicle) on 2.5x2.5 cm of the clipped dorsal skin under semi-occlusion for 4 hours.
Remarks: Observations: Skin observations at 24, 48 and 72 h after application.

Results

Result: not irritating
Primary Dermal Irritation Index (PDII): n/a
Remarks: No irritation was observed; all scores were "0".

Data Quality

Reliability (Klimisch): 2
Remarks: Reliable with restrictions. Not GLP.
Flag Critical study for SIDS endpoint

Reference

Source Reference: 14. Huels AG, Marl, Germany. Prüfung der akuten Hautreizwirkung von Na-Cumolsulfonat / 0020. 1982c

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory: Hüls AG, Prüfinstitut für Toxikologie, Marl, Germany
Print File Name: 5.2.1_28348-53-0_47
Last Revised: 11-04-2005
Remarks: Appears to be the same study reported in 1995 IUCLID reference and in 1994 Greim et al reference.

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: not indicated

Remarks: n/a

Method

GLP: no

Report/Study Year: 1981

Report/Study Number: SDAHT05

Method/Guideline Followed: OECD Guideline 404

Analytical Monitoring: n/a

Species: Rabbit

Remarks: No details provided.

Results

Result: not irritating

Primary Dermal Irritation Index (PDII): n/a

Remarks: n/a

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 10. Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate. 1995

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name: 5.2.1_28348-53-0_60

Last Revised: 6-29-2004

Remarks: Appears to be the same study reported in 1982c Huels reference and in 1994 Greim et al. reference.

Test Substance

CAS Number: 28348-53-0

Identity: Cumene sulfonic acid, sodium salt

Purity: Not indicated

Remarks: n/a

Method

GLP: n/a
Report/Study Year: n/a
Report/Study Number: SDAHT01
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Species: Rabbit
Remarks: No details

Results

Result: not irritating
Primary Dermal Irritation Index (PDII): n/a
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Publication lacks study details.

Reference

Source Reference: 7. Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.1_28348-53-0_62
Last Revised: 6-29-2004
Remarks: Appears to be the same study reported in 1995 IUCLID reference and in 1982c Huels reference.

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: n/a

Analytical Monitoring: n/a
Species: New Zealand Albino Rabbit
Vehicle: n/a
Number of Animals: not indicated
Concentration: 1% active
Exposure: n/a
Remarks: undiluted

Results

Result: mild to moderate
Primary Dermal Irritation Index (PDII): n/a
Remarks:

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.1_28348-53-0_129
Last Revised: 7-20-2004
Remarks: n/a

5.3.B EYE IRRITATION

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: 96.0%
Remarks: Chemical substance is verified, but not CAS number, in original report

Method

GLP: no
Report/Study Year: 1982
Report/Study Number: 0021
Method/Guideline Followed: OECD 405
Species: Rabbit (Small White Russian), weight 2.0-2.4 kg
Vehicle: n/a

Number of Animals: 3 males and 3 females.

Dose: 50 mg

Remarks: Dosage: Application of 50 mg into the conjunctival sac of one eye. Observations: Eye readings 1, 24, 48 and 72 hours after application, additional readings until no symptoms occurred.

Results

Result: Not irritating

Remarks:

Animal	1				2				3				4				5				6			
Effect	C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj	
Time			Red	Ch			Red	Ch			Red	Ch			Red	Ch			Red	Ch			Red	Ch
1 h *	1	0	1	1	1	0	1	1	1	0	1	1	1	0	1	3	1	0	1	1	1	0	1	2
24 h *	1	1	2	1	1	1	1	1	1	1	1	0	1	1	1	2	1	1	2	1	1	1	1	0
48 h *	1	0	1	0	1	1	1	0	1	0	<1	0	1	<1	1	1	1	0	1	0	1	0	<1	0
72 h	1	0	0	0	1	0	<1	0	1	0	0	0	1	0	1	0	1	0	<1	0	1	0	0	0
6 d	0		0	0	1		0	0	1		0	0	1		0	0	0		0	0	0		0	0
8 d	0				0				0				1				0				0			

* Discharge was seen among animals C=corneal opacity I=Iris Conj=conjunctiva Red=redness Ch=chemosis

Not irritating to the eyes.

Minor remark. In one animal an effect on the cornea was present on day 8. No effect was present at the end of the observation period (14 days). According to OECD 405 the observation period should be sufficient to evaluate possible reversibility of the effects. In view of the effect seen and the incidence of the effects, it is considered that this OECD criterium was met.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Non GLP.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 13. Huels AG, Marl, Germany. Prüfung der akuten Augen- und Schleimhautreizwirkung von Na-Cumolsulfonat / 0021. 1982b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Hüls AG, Prüfinstitut für Toxikologie, Marl, Germany

Print File Name: 5.2.2_28348-53-0_49

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1981
Report/Study Number: SDAHT05
Method/Guideline Followed: OECD Guideline 405
Species: rabbit
Vehicle: n/a
Number of Animals: n/a
Dose: n/a
Remarks: 60% solution

Results

Result: not irritating
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 10. Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate. 1995

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.2_28348-53-0_61
Last Revised: 11-04-2005
Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: Not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: n/a
Report/Study Number: SDAHT01
Method/Guideline Followed: not indicated
Species: n/a
Remarks: No details provided.

Results

Result: not irritating
Remarks: n/a

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Publication lacks study details.

Reference

Source Reference: 7. Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.2_28348-53-0_63
Last Revised: 6-22-2004
Remarks: n/a

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: Not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Species: Rabbits
Vehicle: n/a
Number of Animals: 3 per treatment

Dose: n/a
Remarks: Treatments included "undiluted - non-rinsed and rinsed" and 10% aqueous solution - non-rinsed and rinsed.

Results

Result: Irritating
Remarks: Undiluted, non-rinsed treatments produced relatively severe ocular involvement which failed to clear in one eye within the 35-day period of observations. Rinsing reduced involvement to transient, slight to moderate levels. Dilution further reduced ocular involvement so that transient slight effects were the only signs produced.

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.2.2_28348-53-0_130
Last Revised: 6-22-2004
Remarks: n/a

5.4 SENSITIZATION

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: not indicated
Remarks: n/a

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Analytical Monitoring: n/a
Test Type: Human repeat insult patch test
Vehicle: n/a
Number of Animals: 75
Species: Human subjects

Concentration: 0.5% aqueous solution of diluted granular laundry detergent product
Remarks: n/a

Results

Result: not sensitizing
Remarks: No evidence of skin sensitization

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.3_28348-53-0_69
Last Revised: 6-22-2004
Remarks: n/a

5.5 REPEATED DOSE TOXICITY

Test Substance

CAS Number: 28348-53-0
Identity: Cumene sulfonic acid, sodium salt
Purity: 42.3%
Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: No
Report/Study Year: 1968
Report/Study Number: V2781-1
Method/Guideline Followed: not indicated; resembles OECD 408
Analytical Monitoring: n/a
Test Type: 91-day rat feeding study
Species: Rat
Strain: CD
Sex: Male/female
No. of animals 20 per sex per dose group

Route of Administration:	diet
Exposure Period:	13 weeks
Doses:	0, 0.005, 0.05 and 0.5 % in diet.
Control Group:	yes
Frequency of Treatment:	diet
Post Exposure Observation Period:	n/a
Remarks:	Observations: Feed consumption and body weight gain in all animals; 5 animals/sex/dose level were necropsied. On these animals blood parameters, macroscopic examination and histopathology were reported.

Results

Value: NOAEL = 15 mg/kg bw/day active ingredient for females and >114 mg/kg bw/day active ingredient for males

Results:

Dose (% in diet)	0		0.005		0.05		0.5		DR	
Actual mean dose admin. (mg/kg bw/day)	0	0	1.1	1.5	11	15	114	159		
Sex	M	F	M	F	M	F	M	F	M	F
MORTALITY	None									
Clinical signs	Not reported									
Body weight gain								dc		x
Food consumption	No treatment related effects									
Haematology										
HB				ic						
Organ weight										
Liver				ic[r]						
Necropsy	No treatment related effects									
Histopathology(A)	No treatment related effects									

(A) No lesions were found that were considered to be treatment related. Five animals were necropsied per sex per dose. Severe tubule atrophy and degeneration had occurred in the testes of one animal treated at the highest dose. Similar but a mild lesion was seen in one male treated with 0.05% test substance. Histopathology confirmation study took tissues from 4 additional controls rats and 12 treated rats (presumably 4 males from each dose). No lesions attributable to the treatment were evident.

Prostatitis was observed in two animals in the low dose group, and no dose response effect was seen. The authors stated that there was also a slight increase in the number of animals (numbers were not reported) with the pulmonary lesions common to the rat (i.e. perivasculitis and peribronchitis), however, there was no difference in the incidence

between the control and treated rats. All but 5 rats had murine pneumonia in the histopathology confirmation study.

DR = dose related (indicated with an "x")
ic = significant increase
dc = significant decrease
r = relative to body weight

Remarks:
1. In this limited report no information is present on (initial) body weight, clinical observations and clinical chemistry. Limited haematology (no bloodclotting potential), macroscopy and histopathology were performed on 5 animals/sex only.
2. The lowered body weight gain seen in females at the highest dose level (11.7% decreased compared to controls) was stated to remain within the established ranges for animals of this age and species and was not associated with any histopathologic or other effects; however since the change was greater than 10% it can be considered a slight toxic effect that is likely very close to a NOAEL. The intervals between the doses are large (10X) and therefore the only assignable NOAEL is 15 mg/kg bw/day.
3. The increased haemoglobin level seen females at the lowest dose group and the decreased relative liver weight in males of the same group are considered to be unrelated to treatment as the effects were not seen in the opposite sex and no dose response relationship for these effects could be established.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Limited report, large intervals between doses, and no analyses or information on impurities in the test substance.

Reference

Source Reference: 18. Procter & Gamble Company. 91-Day rat feeding study. 1968

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Procter & Gamble Research Division

Print File Name: 5.4_28348-53-0_83

Last Revised: 11-04-2005

Remarks:
1. The intervals between the dose levels in this study are large (factor 10). OECD 408 prefers 2-4 fold intervals and prefers an additional group if the factors are > 6-10.
2. No information was given on diet preparation and storage. No analyses of accuracy of preparation and of stability under storage conditions were performed. Impurities in the test substance formulation are unknown.

5.6 GENETIC TOXICITY *IN VITRO*

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt; Na cumene sulfonate
Purity:	40% active ingredient
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	no data
Report/Study Year:	1984
Report/Study Number:	840126
Method/Guideline Followed:	OECD Guideline 471
Test Type:	Ames Test
System:	*Salmonella typihimurium*
Test Concentration:	3.2, 16, 80, 400 and 2000 µg active ingredient
Species/strain:	TA 1535; TA 100; TA 1537; TA 1538; TA98
Metabolic Activation:	with and without S-9 mix
Remarks:	Positive controls (no metabolic activation): sodium-azide for TA 1535 and TA 100. 4-nitro-o-phenylenediamine for TA 1537, TA 1538 and TA 98. Positive control (with metabolic activation): 2-aminoanthracene, all strains. Negative control: vehicle (water), all strains.

Results

Result:	Negative; not mutagenic
Cytotoxic Concentration:	not cytotoxic at highest dose
Remarks:	n/a.

Data Quality

Reliability (Klimisch):	1
Remarks:	Reliable without restriction, guideline study.
Flag	Critical study for SIDS endpoint

Reference

Source Reference:	8. Henkel KGaA, Dusseldorf, Germany, Natriumcumolsulfonat. Prüfung auf Mutagenität in Ames-Test. 840126. 1984a

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	Henkel KGaA, Department of Toxicology

Print File Name:	5.5_28348-53-0_161
Last Revised:	11-04-2005
Remarks:	n/a

5.7 GENETIC TOXICITY *IN VIVO*

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt
Purity:	99.4%
Remarks:	40% solution in water

Method

GLP:	yes
Report/Study Year:	1992
Report/Study Number:	MK-91/0029
Method/Guideline Followed:	OECD 474 (1983), EEC 84/449 L251
Test Type:	Mouse micronucleus cytogenetic assay
Species:	Mouse , 24-30 g.
Strain:	NMRI
Sex:	Male/female
No. of animals	5 per sex per dose group per sample time
Route of Administration:	Oral gavage
Exposure Period:	Single dose
Doses:	Single oral dose at 0 and 4467 mg/kg bw; vehicle water, dose volume 17 ml/kg bw. Dose selection was based on preliminary studies with 2-5/sex: no deaths at and below 4467 mg/kg bw (one incidental death (female) at 3981 mg/kg bw), 4/10 deaths at 5000 mg/kg bw.
Remarks:	Statistical Method: Chi^2 test Sampling times: 24, 48 and 72 hours post-dose. Positive control: Cyclophosphamid Scoring: For each animal, the following proportions were determined in bone marrow smears: • PolyChromatic Erythrocytes (PCE)/ NormoChromatic Erythrocytes (NCE) in 1000 erythrocytes. • Micronucleated PolyChromatic Erythrocytes (MPCE) per 1000 PCE. • Micronucleated NormoChromatic Erythrocytes (MNCE) in

NormoChromatic Erythrocytes (NCE).

Results

Result: Not clastogenic

Results:

Dose [mg/kg bw]/effect	0		4467		DR
Sex	M	F	M	F	
Mortality			0/15	0/15	
Clinical signs(A)			+	+	
PCE/NCE (72 h)				(dc)	
MPCE [% of PCE] (72 h)				(ic)	
MNCE [% of NCE]	Not reported				

(A) The clinical signs observed included piloerection, hunched posture, diarrhoea and closed eyes.

Abbreviations: DR = dose related; dc = significant decrease; ic = significant increase; + = presence

Positive control gave the expected results.

Remarks:

- The number of micronucleated polychromatic erythrocytes was slightly, but significantly increased in females sacrified after 72 hours. Since no similar effect was seen in males and the ratio PCE/NCE was lowered, which is considered to be a sign of bone marrow toxicity, no toxicological significance was attributed to this effect.
- The proportion of MPCE was determined for 1000 PCE. This is in agreement with OECD 474 (1983); OECD 474 (1997) requires evaluation of 2000 PCE.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 12. Huels AG, Marl, Germany. Mikrokerntest mit Natrium-Cumol-sulfonat an der Maus / MK-91/0029. 1992

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Hüls AG, Prüfinstitut für Toxikologie, Marl, Germany

Print File Name: 5.6_28348-53-0_70

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number:	28348-53-0
Identity:	Cumene sulfonic acid, sodium salt; Na-cumene sulfonate
Purity:	40%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	no data
Report/Study Year:	1984
Report/Study Number:	840241
Method/Guideline Followed:	OECD Guideline 474
Test Type:	Mouse micronucleus cytogenetic assay
Species:	Mouse, approx. 8 weeks old, 25 - 30 g.
Strain:	Albino CF1/W68
Sex:	male/female
No. of animals	7 per sex per dose
Route of Administration:	oral
Exposure Period:	30 hours
Doses:	1000, 5000 and 10000 mg/kg bw in two equal applications 24 hours apart
Remarks:	Statistical method: Kastenbaum-Bowman Tables. First dose at 0 hours, second dose at 24 hours. Vehicle: doses administered in 10 ml ddH_2O. Negative vehicle control (2 x 10 ml ddH_2O). Positive control: Endoxan® (intra-peritoneal, 2 x 10 mg/kg bw) Sampling time: 30 hours. Scoring: For each animal, the following proportions were determined in bone marrow smears: • PolyChromatic Erythrocytes (PCE) in 1000 erythrocytes. • Micronucleated PolyChromatic Erythrocytes (MPCE) per 1000 PCE. • Micronucleated NormoChromatic Erythrocytes (MNCE) per 1000 PCE. • MNCE/MPCE ratio.

Results

Result: Not clastogenic

Result: Positive control: Endoxan® (i.p. 2 x 10 mg/kg bw) gave the expected response.

Dose [mg active ingredient/kg bw]/effect	0	1000	5000	10000	DR
Mortality	1 each sex, highest dose				
[MNCE/MPCE]	no treatment related effects				

. DR = dose related as indicated by "x"

Remarks: *Minor remark*: The MNCE/MPCE ratio was determined for 1000 PCE. This is in agreement with OECD 474 (1983); OECD 474 (1997) requires evaluation of 2000 PCE.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction, guideline study.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 9. Henkel KGaA, Dusseldorf, Germany, Natriumcumolsulfonat. Prüfung auf Mutagenität in Mikrokern-Test in vivo, 840241, 1984b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Henkel KGaA, Department of Toxicology

Print File Name: 5.6_28348-53-0_160

Last Revised: 11-04-2005

Remarks: n/a

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Albright & Wilson Americas Inc., Glen Allen, Virginia, USA. Material Safety Data Sheet Eltesol SC 93 / MSDS Ref No.: PSMSD-287. 1997

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Greim, H., J. Ahlers, R. Bias, B. Broecker, H. Hollander, H.-P. Gelbke, H.-J. Klimisch, I. Mangelsdorf, A. Paetz, N. Schön, G. Stropp, R. Vogel, C. Weber, C. Ziegler,-Skylakakis and E. Bayer. 1994. Toxicity and Ecotoxicity of Sulfonic Acids: Structure Activity Relationship. Chemosphere 28(12): 2203-2236

Henkel KGaA, Dusseldorf, Germany, Natriumcumolsulfonat. Prüfung auf Mutagenität in Ames-Test. 840126. 1984a

Henkel KGaA, Dusseldorf, Germany, Natriumcumolsulfonat. Prüfung auf Mutagenität in Mikrokern-Test in vivo, 840241, 1984b

Huels AG, Marl, Germany. Akute orale Toxizität von Na-Cumolsulfonat / 0019. 1982a

Huels AG, Marl, Germany. Prüfung der akuten Augen- und Schleimhautreizwirkung von Na-Cumolsulfonat / 0021. 1982b

Huels AG, Marl, Germany. Prüfung der akuten Hautreizwirkung von Na-Cumolsulfonat / 0020. 1982c

Huels AG, Marl, Germany. Mikrokerntest mit Natrium-Cumol-sulfonat an der Maus / MK-91/0029. 1992

Huels AG, Germany. IUCLID Data Sheet Sodium Cumenesulphonate. 1995

Mackay D., A. DiGuardo, S. Paterson and C. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environmental Toxicology and Chemistry (15) 9: 1627-1637

Procter & Gamble Company. 91-Day rat feeding study. 1968

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA, Acute toxicity of sodium cumene sulfonate to *Daphnia magna* / 40423. 1992b

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA; Statis acute toxicity of sodium cumene sulfonate to fathead minnow (Pimephales promelas) / 40421. 1992e

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Aerobic biodegradation of sodium cumenesulfonate in the modified Sturm test / 40427. 1993

Rütgers Organics Corporation, State College, Pennsylvania. Material Safety Data Sheet Naxonate® SC / MSDS No. 1-10100. 1997c

The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 – 1978

Trent University Canadian Environmental Modeling Centre at www.trentu.ca/cemc/welcome.html

Witco Chemical Corporation, Paterson, New Jersey, USA letter to Soap & Detergent Association (dated September 26, 1977) summarizing study data

SIDS DOSSIER

CAS NO. 37475-88-0

Cumene sulfonic acid, ammonium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
12068-03-0
16106-44-8
26447-10-9
28088-63-3
28348-53-0 (32073-22-6)
30346-73-7

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **37475-88-0**

B. Name *(IUPAC name)* **ammonium cumenesulphonate**

C. Name *(OECD name)* **cumene sulfonic acid, ammonium salt**

D. CAS Descriptor **Benzenesulfonic acid, (1-methylethyl)-, ammonium salt**

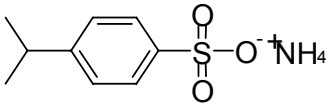
E. EINECS-Number **253-519-1**

F. Molecular Formula **C9 H15 N1 O3 S1**

G. Structural Formula

Commercial cumene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the para isomer as a representative structure. An ortho-isomer would have adjacent attachment points on the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.

.



H. Substance Group **Hydrotropes category**

I. Substance Remark

J. Molecular Weight **217 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country: Australia

B. Lead Organization:

Name of Lead Organization:

National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
Tel: +61 2 8577 8880

C. Name of responder

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USA

Name: Lionel Godefroy
Address:
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Chemin Jongkind
38340 Voreppe
France

1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six “sponsored” substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate.

1.2 SYNONYMS

cumenesulfonic acid, ammonium salt
cumenesulfonate, ammonium salt
ammonium cumene sulfonate
benzenesulfonic acid (1-methylethyl) ammonium salt
methylethylbenzenesulfonate, ammonium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%
Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number:	37475-88-0
Identity:	Cumene sulfonic acid, ammonium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: CC(C)c1ccc(S(=O)(=O)ON(H)(H)(H)H)cc1 MOL FOR: C9 H15 N1 O3 S1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	EPI-001
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	217.28	
Water Solubility (mg/l):	2.246e+004	n/a
Octanol Water Partition Coefficient (Log Kow):	0.23	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	472.53	n/a
Melting Point (°C):	199.77	n/a
Vapor Pressure(mmHg):	1.93E-009	n/a
Henry's Law Constant (atm/(mole/m^3)):	2.457E-014	n/a
Atmospheric Oxidation Half-Life (hours):	39.5	n/a
Soil Adsorption Coefficient (Log Koc):	3.164	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.0.1_37475-88-0_166
Last Revised:	11-04-2005
Remarks:	n/a

2.1 MELTING POINT

Modeled melting point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Melting point was measured for CAS numbers 12068-03-0, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

2.2 BOILING POINT

Modeled boiling point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Boiling point was measured for CAS numbers 1300-72-7 and 26447-10-9.

2.3 DENSITY

Density was measured for CAS numbers 28088-63-3 and 1300-72-7 (827-21-4).

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW})

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. $\log_{10} K_{ow}$ was measured for CAS number 28088-63-3.

2.6.1 WATER SOLUBILITY & DISSOCIATION CONSTANT

Modeled water solubility is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Solubility was measured for CAS numbers 1300-72-7 (827-21-4), 12068-03-0, 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

3.0.1 EQC MODEL

Fugacity modelling has been conducted on CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	37475-88-0
Identity:	Cumene sulfonic acid, ammonium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: CC(C)c1ccc(S(=O)(=O)ON(H)(H)(H)H)cc1 MOL FOR: C9 H15 N1 O3 S1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 37475880
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	3.26 E-12 cm3/molecule-sec
Half Life	39 hrs
Remarks:	n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File	AOPWOO1 37475880

Name:
Last Revised: 05-09-06
Remarks: n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

Refer section 3.0.1 EQC Model.

3.4 BIODEGRADATION

Biodegradation data are available for CAS numbers 1300-72-7(827-21-4), 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6).

3.6 BIOACCUMULATION

Estimated data is available for this CAS number in EPISuite estimation of Physical/Chemical Properties in 2.0.1. Measured data is available for CAS numbers 12068-03-0 and 1300-72-7 (827-21-4).

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Fish toxicity data are available for CAS numbers 1300-72-7(827-21-4), 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2A ACUTE ORAL TOXICITY

Acute oral toxicity data are available for CAS numbers 1300-72-7(827-21-4), 12068-03-0, 16106-44-8, 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

5.2.B ACUTE INHALATION TOXICITY

Acute inhalation toxicity data are available for CAS numbers 12068-03-0, 26447-10-9 and 28348-53-0 (32073-22-6).

5.2.C ACUTE DERMAL TOXICITY

Acute dermal toxicity data are available for CAS Nos 28088-63-3 and 28348-53-0 (32073-22-6).

5.3.A SKIN IRRITATION

Skin Irritation/Corrosion data are available for CAS numbers 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.3.B EYE IRRITATION

Eye Irritation/Corrosion data are available for CAS numbers 16106-44-8, 12068-03-0, 28088-63-3, 26447-10-9, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.4 SENSITIZATION

Skin sensitization data are available for CAS numbers 12068-03-0, and 28348-53-0 (32073-22-6).

5.5 REPEATED DOSE TOXICITY

Repeated dose toxicities were measured for CAS Nos 1300-72-7 (827-21-4) and 28348-53-0 (32073-22-6).

5.6 GENETIC TOXICITY *IN VITRO*

Genetic toxicity (*in vitro*) data were collected for CAS numbers 1300-72-7 (827-21-4) and 28088-63-3, and 28348-53-0 (32073-22-6).

5.7 GENETIC TOXICITY IN VIVO

Genetic toxicity (in vivo) data were collected for CAS Nos 28088-63-3, and 28348-53-0 (32073-22-6).

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

SIDS DOSSIER

CAS NO. 28088-63-3

Xylene sulfonic acid, calcium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
12068-03-0
16106-44-8
26447-10-9
28348-53-0 (32073-22-6)
30346-73-7
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **28088-63-3**

B. Name (IUPAC name) **calcium xylenesulphonate**

C. Name (OECD name) **xylene sulfonic acid, calcium salt**

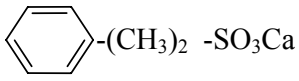
D. CAS Descriptor **Benzenesulfonic acid, dimethyl-, calcium salt**

E. EINECS-Number **248-829-9**

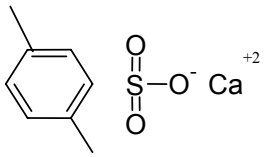
F. Molecular Formula **C8 H9 O3 S1 Ca1**

G. Structural Formula

Commercial xylene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the meta, ortho isomer as a representative structure. A para-isomer would have attachments at opposite ends of the benzene ring, a meta-isomer would have one open carbon between attachments on the benzene ring, and an ortho isomer would have adjacent attachment points on the benzene ring..



.



H. Substance Group **Hydrotropes category**

I. Substance Remark

J. Molecular Weight **217 grams/mole**

1.02 OECD INFORMATION

5.1.1 A. Sponsor Country: **Australia**

5.1.2 B. Lead Organization:

Name of Lead Organization:
National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
Tel: +61 2 8577 8880

C. Name of responder

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Fax: (202) 347-4110

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France

1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six "sponsored" substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

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The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate or

1.2 SYNONYMS

xylenesulfonic acid, calcium salt

xylenesulfonate, calcium salt
calcium xylene sulfonate
benzenesulfonic acid (1-dimethyl) calcium salt
dimethylbenzenesulfonate, calcium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%

Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITETM ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt

Purity: n/a

Carbon Chain Length Distribution: n/a

Remarks: SMILES: [Ca]OS(=O)(=O)c1ccc(cc1C)C
MOL FOR: C8 H9 O3 S1 Ca1

Method

GLP: n/a

Report/Study Year: n/a

Report/Study Number: EPI-001

Method/Guideline Followed: n/a

Remarks: n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	217.21	
Water Solubility (mg/l):	1e+006	n/a
Octanol Water Partition Coefficient (Log Kow):	-1.92	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	544.57	n/a
Melting Point (°C):	247.42	n/a
Vapor Pressure(mmHg):	1.2E-011	n/a
Henry's Law Constant (atm/(mole/m^3)):	3.123E-018	n/a
Atmospheric Oxidation Half-Life (hours):	41	n/a
Soil Adsorption Coefficient (Log Koc):	1.500	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions

Reference

Source Reference: Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Other References: n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.0.1_28088-63-3_163
Last Revised:	11-4-2005
Remarks:	n/a

2.1 MELTING POINT

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA
Purity:	not indicated
Carbon Chain Length Distribution:	n/a
Remarks:	While the testing laboratory was blinded as to the identity of the test substance, the test sponsor confirms that the test substance was xylene sulfonic acid, calcium salt.

Method

GLP:	yes
Report/Study Year:	1997
Report/Study Number:	41810
Method/Guideline Followed:	OECD 102
Analytical Monitoring:	n/a
Remarks:	The melting temperature was electronically determined using the change in light transmission through a sample as it passed from the solid phase to the liquid phase. The determination of the melting temperature by the instrument is based on the principle of the Thiele Tube technique.

Results

Remarks: No melting point was observed over the range from 100 °C to 375 °C. The test substance underwent a color change from white to dark grey, indicating decomposition.

The melting point could not be determined due to decomposition of the substance.

A 2nd determination was performed and the same results were obtained.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 42 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of the melting temperature of SS0335.01 / 41810. 1997a

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	ABC Laboratories Inc., Colombia, Missouri, USA
Print File Name:	2.1_28088-63-3_110
Last Revised:	11-04-2005
Remarks:	n/a

2.2 BOILING POINT

Modeled boiling point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Boiling point was measured for CAS numbers 1300-72-7 and 26447-10-9.

2.3 DENSITY

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA
Purity:	not indicated
Remarks:	While the testing laboratory was blinded as to the identity of the test substance, the test sponsor confirms that the test substance was xylene sulfonic acid, calcium salt.

Method

GLP:	yes
Report/Study Year:	1996
Report/Study Number:	41812
Method/Guideline Followed:	OECD 109
Test Type:	n/a
Temperature (°C):	20.2 ± 0.4
Remarks:	Gas Pycnometer. Measurement was performed in triplicate.

Results

Value: Measurement 1: 1.2945 ± 0.0008 g/cm^3
Measurement 2: 1.3007 ± 0.0012 g/cm^3
Measurement 3: 1.3048 ± 0.0009 g/cm^3
Mean: 1.300 ± 0.0052 g/cm^3

Remarks:

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 28. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of the density of SS0335.01 / 41812. 1996

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 2.3_28088-63-3_113

Last Revised: 11-04-2005

Remarks: n/a

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate, Ca

Purity: not indicated

Remarks: The identity of SS0335.01 could not be verified from the study report.

Method

GLP: yes

Report/Study Year: 1997

Report/Study Number: 41814

Method/Guideline Followed: OECD 107 (1995). Shake Flask

Analytical Monitoring: yes

Temperature °C: 21 ° C

Remarks: Six test systems were prepared by transferring 100 mL of octanol saturated with deionised water to individual amber bottles. Duplicate systems at three dosing levels were prepared by transferring 2.0 mL of a 0.953 mg/mL dosing solution (SS0335.01 in water saturated with octanol) to two bottles, 4.0 mL of the dosing solution to two bottles and 8.0 mL of the dosing solution to two bottles. The sealed bottles were placed on a shaker at 21 ± 1 °C for 24 hours. Duplicate aliquots of ca. 40 mL were removed from the octanol phase of the three dose level systems and centrifuged (10000 rpm, 30 min, 21 °C). Aliquots of 35 mL from each centrifuge tube were extracted three times with 5.0 mL of water saturated with octanol (one minute per extraction). The final volumes were adjusted to 15 mL with additional water saturated with octanol. Duplicate aliquots were removed from the aqueous layers of the three dose level systems with glass syringes and centrifuged (10000 rpm, 30 min, 21 °C). An aliquot of 0.25 mL of each aqueous sample was diluted to 10 mL with water saturated with octanol. The diluted aqueous samples were analysed by HPLC.

The pH of each of the remaining aqueous samples was measured.

Results

Log P_{ow}: -2.69 to -2.71

Remarks:

Sample	concentration [mg/mL]	Pow	^{10}log(Pow), mean
2.0 mL dose, repl. 1, octanol	0.00175	0.00200	-2.71
2.0 mL dose, repl. 1, water	0.877		
2.0 mL dose, repl. 2, octanol	0.00171	0.00194	
2.0 mL dose, repl. 2, water	0.880		
4.0 mL dose, repl. 1, octanol	0.00181	0.00200	-2.70
4.0 mL dose, repl. 1, water	0.903		
4.0 mL dose, repl. 2, octanol	0.00181	0.00198	
4.0 mL dose, repl. 2, water	0.914		
8.0 mL dose, repl. 1, octanol	0.00183	0.00198	-2.69
8.0 mL dose, repl. 1, water	0.926		
8.0 mL dose, repl. 2, octanol	0.00194	0.00211	
8.0 mL dose, repl. 2, water	0.921		

^{10}log(Pow) of SS0335.01 was calculated to be –2.70 ± 0.01

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 30. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of the octanol/water partition coefficient (Shake Flask Method) of SS0335.01 / 41814. 1997b

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 2.5_28088-63-3_111

Last Revised: 11-04-2005

Remarks: n/a

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate, Ca

Purity: not indicated

Remarks: The identity of SS0335.01 could not be verified from the study report

Method

GLP: yes

Report/Study Year: 1997

Report/Study Number: 41813

Method/Guideline Followed: OECD guideline 105 (1995). Shake Flask

pH: 6.67

Remarks: Saturated aqueous samples were generated by first equilibrating an excess of test substance (ca. 3 grams) at approximately 30 °C with deionized water (2 mL) for ca. 18 hours. One replicate sample was then placed on a tumbler, submerged in a water bath at 20 ± 1 °C for 24 hours prior to analysis. Solid and aqueous phase separation was achieved by centrifugation (>=39000g, 30 minutes, 20 °C). Duplicate 100 µL subsamples were removed from the filtered supernatant and diluted to a final volume of 100 mL with deionized water. Dilutions of these solutions (10* diluted) were used for HPLC analysis with UV detection. The 2nd and 3rd replicates were equilibrated for 2 and 3 days respectively with sampling and analysis as above, conducted every 24 hours.

An external calibration curve was prepared by analyzing standard solutions of the test substance.

Results

Value: 553 g/l at 20 °C

Remarks:

Sample	Concentration (g/L)	Mean concentration (g/L)	% Change
Day 1, replicate 1	551		
Day 1, replicate 2	547	549	-
Day 2, replicate 1	553		
Day 2, replicate 2	555	554	0.911
Day 3, replicate 1	556		
Day 3, replicate 2	558	557	0.542

The test substance was considered to be at equilibrium when the concentration in the reagent water between at least the last two sampling days was less than 15%.

The pH values of the saturated aqueous solutions were 6.84, 6.57 and 6.61 for the Day 1, Day 2 and Day 3 samplings, respectively.

The solubility of SS0335.01 in deionized water was determined to be 553 ± 4 g/L at 20 ± 1 °C.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 31. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of water solubility (shake flask method) of SS0335.01 / 41813. 1997c

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 2.6.1_28088-63-3_112

Last Revised: 11-04-2005

Remarks: n/a

3.0.1 EQC MODEL

Test Substance

CAS Number: 28088-63-3

Identity: Cumene sulfonic acid, sodium salt

Purity: n/a

Remarks: n/a

Method

Report/Study Year: 2003

Report/Study Number: SDAHT10

Method/Guideline Followed: Fugacity Level III; version 2.02

Test Type: modelling

Media: n/a

Remarks: Input parameters were based on measured or EPIWIN-modelled physico-chemical properties of the test material. Water solubility = 553,000 mg/L; octanol water partition coefficient = -2.7; melting point = 375 ^{o}C; vapor pressure = 1.2 x 10^{-11}.
Total mass used as release volume = 3310.5 kg/h to water (based on 29,000 tonnes released over 356 days, 24 hours per day). Emission levels used for Level II modeling would be the default 1000 kg/h to water, air, sediment.

Results

	Air (%)	Water (%)	Soil (%)	Sediment (%)
Level III	0	99.9	0.1	0

Remarks: The outputs for both Level II and III are almost identical.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Modelling estimate based on some measured and some estimated input parameters.

Flag Critical study for SIDS endpoint

Reference

Source Reference: Trent University Canadian Environmental Modeling Centre at www.trentu.ca/cemc/welcome.html.

Other References: Mackay D., A. DiGuardo, S. Paterson and C. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environmental Toxicology and Chemistry (15) 9: 1627-1637.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Print File Name:	3.3.1_28088-63-3_119
Last Revised:	11-04-2005
Remarks:	n/a

3.1.A PHOTODEGRADATION

Modeled photodegradation data is available for CAS numbers 12068-03-0, 1300-72-7 (827-21-4), 16106-44-8, 26447-10-9, 28348-53-0 (32073-22-6), 30346-73-7, and 37475-88-0.

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

Refer section 3.0.1 EQC Model.

3.4 BIODEGRADATION

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA
Purity:	31.2%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	yes
Report/Study Year:	1994
Report/Study Number:	41654
Test Type:	aerobic
Method/Guideline Followed:	OECD 301B. Modified Sturm Test
Inoculum:	activated sludge
Inoculum Acclimated:	yes
Acclimated to what Concentration:	20 mg C/L
Acclimated for what Duration:	19 days

Control Substance: Sodium benzoate

Test Substance Initial Concentration:

Value	Unit	Expressed as
10	mg/L	OrganicCarbon (OC)
20	mg/L	OC

Control Substance Initial Concentration:

Value	Unit	Expressed as
20	mg/L	OC

Remarks:

- Pre-acclimation phase: none
- Temperature: 20 - 22 °C.
- Analysis: CO_2 produced was trapped in 0.2N KOH solutions in the gas-washing bottles.
- Analysis on day 3, 6, 9, 15, 16, 19, 23, 25 and 29.
- Test substance was tested in duplicate bottles.

Results

Results:

results in %$THCO_2$

day	3	6	9	15	16	19	23	25	29
10 mg Carbon/L	0	28.33	48.53	54.17	55.92	67.54	73.10	75.77	83.64
10 mg C/L	0	33.50	50.81	55.07	56.03	57.56	67.49	73.02	87.47
20 mg C/L	0	25.96	50.15	56.83	57.96	60.30	63.14	64.56	81.75
20 mg C/L	0	21.87	43.80	46.65	47.05	47.86	55.93	60.96	68.64
Reference	44.80	72.43	79.53	88.93	90.83	94.40	99.90	102.8	112.9

The substance can be classified as moderately to ready biodegradable, more than 60% after 19-25 days.

Remarks:

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 27. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. CO_2 evolution test (Modified Sturm Test) with Calcium Xylenesulfonate. 1994f

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 3.5_28088-63-3_98

Last Revised: 11-04-2005

Remarks: n/a

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt. Dimethylbenzenesulfonate CA
Purity:	31.2%
Remarks:	Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	yes
Report/Study Year:	1994
Report/Study Number:	41655
Test Type:	removability
Method/Guideline Followed:	OECD 302A. Semi-Continuous Activated Sludge Removal
Inoculum:	Activated sludge
Inoculum Acclimated:	yes
Acclimated to what Concentration:	4 mg Carbon/L for four days, then 20 mg C/L from day five forward.
Acclimated for what Duration:	7 days
Control substance:	None

Test Substance Initial Concentration:

Value	Unit	Expressed as
20	mg/L	OrganicCarbon

Remarks:

- Inoculum: activated sludge collected from aeration pool of the Colombia Wastewater Treatment Facility in Columbia, Missouri, USA. The suspended solids were concentrated by allowing the sludge to settle and then siphoning off and discarding approximately half of the total volume of supernatant. The remaining liquid, including half of the supernatant and solids were mixed thoroughly and used directly to charge the acclimation vessel.
- Temperature 20 ± 2 °C.
- Analysis on day 0, 2, 4, 6, and 7.
- Test substance was tested in duplicate bottles, mean given below.

Results

Results: results in % removal

20 mg Carbon/L	85.89	85.46	91.64	95.75	96.77

Remarks: The substance was removed from the test system at an average of 94.72% ± 2.72%.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 34. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Evaluation of potential for removability: the modified semi-continuous activated sludge test with SAR 33-55 / 41655. 1994h

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 3.5_28088-63-3_99

Last Revised: 11-04-2005

Remarks: Total Organic Carbon content at the beginning of the study was 13.75 mg Carbon/L instead of the recommended <12 mg C/L.

3.6 BIOACCUMULATION

Estimated data is available for this CAS number in EPISuite estimation of Physical/Chemical Properties in 2.0.1. Measured data is available for CAS numbers 12068-03-0 and 1300-72-7 (827-21-4).

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate, Ca

Purity: 31.2%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes

Report/Study Year: 1994

Report/Study Number: 41841

Method/Guideline Followed: EPA-TSCA 797.1400

Test Type: acute, flow-through

Analytical Monitoring: yes

Limit Test: n/a

Species: Rainbow Trout (*Oncorhynchus mykiss*) mean length 54 ± 3 mm

Exposure Period:

Value	Unit
96	hour(s)

Remarks: Statistical method: Binominal, moving average and probit analysis.
Number of fish: 10/test vessel, 2 test vessels/treatment.
Concentrations: Nominal: 112, 224, 448, 895 and 1790 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Test conditions: Flow-through without aeration, 6 replacements/24 hours; at 12 ± 1 °C in 15 L glass vessels containing 12 L of medium of hardness 144-146 mg/L (as $CaCO_3$) and pH 8.1; 16 hours light; unfed.
Analyses: From all treatments at 0 and 96 hours by HPLC.
Physical measurements: At 0, 24, 48, 72 and 96 hours: overall ranges for pH 7.7-8.3; O_2 70-83%; temperature 11-13 °C.
Observations: Mortality/symptoms at 24, 48, 72 and 96 hours.
Minor remark. Fish were not fed for 72 hours prior to test initiation rather than 24 hours as stated in OECD 203

Results

Unit: mg/L

Results:

		Mean Measured Concentration (mg/L)					
Parameter	Time [hour]	0	114	227	428	824	1580
Mortality [%]	96	None					
Symptoms*	0-96						+

* Symptoms including loss of equilibrium, surfacing, fish on the bottom, dark discolouration, quiescent and laboured respiration observed as indicated (+).

96-h LC50 >1580 mg/L (equivalent to >490 mg/L active ingredient taking into account the 31% purity of the sample)..

NOEC = 824 mg/L (equivalent to 255 mg/L active ingredient taking into account the 31% purity of the sample).

Remarks: Analyses: Mean measured concentrations 88-102% of nominal; quality control samples (103-1845 mg/L): 94-98%; method recovery (5.25-1050 mg/L): 101% .

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 40 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA; Acute flow-through toxicity of SAR 33-55 to rainbow trout (*Oncorhynchus mykiss*) / 41841, 1994m

Other References: 38 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Validation of analytical methods used in the determination of test concentrations of SAR 33-55 during aquatic toxicity studies / 41658. 1994L.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 4.1_28088-63-3_11

Last Revised: 11-04-2005

Remarks: n/a

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt. Dimethylbenzenesulfonate Ca

Purity: 31.2%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes

Report/Study Year: 1994

Report/Study Number: 41842

Method/Guideline Followed: EPA-TSCA 797.1300

Test Type: acute, flow-through

Analytical Monitoring: yes

Species: *Daphnia magna*, <24 hours old.

Exposure Period:

Value	Unit
48	hour(s)

Remarks: Statistical method: Binominal, moving average and probit analysis.
Number of Daphnids: 10/test vessel, 2 test vessels/treatment.
Concentrations: Nominal: 60, 120, 250, 500 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations not corrected for sample purity.
Test conditions: Flow-through without aeration, 5.6 replacements/24 hours; at 20 ± 2 °C in vessels containing 1 L of medium of hardness 152-154 mg/L (as $CaCO_3$) and pH 8.4; 16 hours light; unfed.
Analyses: From all treatments at 0 and 48 hours by HPLC.
Physical measurements: At 0, 24 and 48 hours: overall ranges for pH 8.2-8.5; O_2 80-89%; temperature 19-21 °C.
Observations: Immobility/symptoms at 24 and 48 hours.

Results

Unit: mg/L

		Mean Measured Concentration (mg/L)					
Parameter	Time [hours]	0	39	150	220	470	1020
Immobility [%]	48	5	5	0	0	0	0
Symptoms*	0-48					+	+

* Daphnids appeared on the bottom of the vessel as indicated (+).

Results: 48-hours EC50 >1020 mg/L (equivalent to >318 mg/L active ingredient taking into account the 31% purity of the sample).

NOEC = 220 mg/L (equivalent to 68 mg/L active ingredient taking into account the 31% purity of the sample).

Analyses: Mean measured concentrations 88-125% of nominal (except for the lowest concentration 65%); quality control samples (41-1025 mg/L): 95-102%; method recovery (5.25-1050 mg/L): 101% .

Remarks: Precipitate was observed in the highest concentration after 48 hours.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 23 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute flow-through toxicity of SAR 33-55 to *Daphnia magna* / 41842. 1994c

Other References: 38 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Validation of analytical methods used in the determination of test concentrations of SAR 33-55 during aquatic toxicity studies / 41658. 1994L.

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 4.2_28088-63-3_19

Last Revised: 11-04-2005

Remarks: n/a

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA

Purity: 31.2%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes

Report/Study Year: 1994

Report/Study Number: 41657

Method/Guideline Followed: EPA-TSCA 797.1050

Analytical Monitoring: yes

Species: Green algae (*Selenastrum capricornutum*).

Endpoint: growth inhibition

Exposure Period:

Value	Unit
96	hour(s)

Remarks: Statistical method: ANOVA (Dunnett).
Initial cell concentration: 10^4 cells/mL.
Three replicates per treatment.

Concentrations: Nominal: 62.5, 125, 250, 500 and 1000 mg/L (no vehicle); untreated controls. Nominal concentrations have not been corrected for sample purity.
Analysis: At 0 hour (single samples) and at 96 hours (in triplicate) from all replicates by HPLC.
Test conditions: 250 mL flasks containing 100 mL of algal medium; temperature: 24 ± 2 °C; continuous illumination (4300 lux); shaken (100 rpm).
Physical measurements: At 0 and 96 hours: overall ranges for pH: 7.4-7.9; temperature 24 °C.
Observations: Cell density at 0, 24, 48, 72 and 96 hours with a haemacytometer.

Results

Unit: mg/L

Results:

		Mean Measured Concentration (mg/L)					
Parameter	Time [hours]	0	60.1	122	240	483	980
Mean cell density [10^4 cells/mL]	0	0.96	1	1	1	1	1
	24	1.8	2.0	1.8	1.1*	1.0*	0.85*
	48	6.1	8.3	5.1	5.6	5.2	3.1*
	72	28	30	25	25	22	13*
	96	100	100	100	94	71*	40*
Inhibition [%] ¨C area under curve	0-96	0	0	5	9	27	59
growth rate	0-96	0	0	0	1	7	20

* Significant effect

96-hour EC50 = 758 mg/L (equivalent to 236 mg/L active ingredient (95% CI 185-288 mg/L based on 31% purity of the substance).
96-hour NOEC 240 mg/L (equivalent to 75 mg/L active ingredient based on 31% purity of the substance).

Analyses: Mean measured concentrations 95-101% of nominal; quality control samples (77-1530 mg/L): 93-100% of nominal.

Remarks:

- Recalculation of the EC50 by the reviewer based on area under the curve (using the 41% trimmed Spearman-Karber method) yielded a 96-hour EC50 value of 803 mg/L (equivalent to 251 mg a.i./l ;95% CI 213-295 mg a.i./L).
- *Minor remark*. Light intensity was only 4000 lux (OECD 201 specifies 8000 lux). Since no effect on algal growth in the control and the low test concentrations was seen, this did not affect the study outcome.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference:	25 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute toxicity of SAR 33-55 to *Selenastrum capricornutum* Printz / 41657, 1994e
Other References:	38 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Validation of analytical methods used in the determination of test concentrations of SAR 33-55 during aquatic toxicity studies / 41658. 1994L.

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	ABC Laboratories Inc., Colombia, Missouri, USA
Print File Name:	4.3_28088-63-3_22
Last Revised:	11-04-2005
Remarks:	n/a

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2.A ACUTE ORAL TOXICITY

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzene sulfonate CA

Purity: 31.2%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: Yes

Report/Study Year: 1994

Report/Study Number: 715-004

Method/Guideline Followed: US EPA TSCA 798.1175

Test type: n/a

Species: Rat

Strain: Crl:CD

Sex: male/female

Vehicle: Deionized water

Number of Animals per Dose: 5/sex/dose group.

Doses: Single oral administration of 2500, 3000, 3300, 3500, 4000 and 5000 mg/kg bw (vehicle water, dosing volume 20 mL/kg); no controls; feeding *ad libitum* (food was withheld ~20 hours prior to dosing and ~3 hours after dosing).

Remarks: Weight 163-248 g
8 weeks of age
Statistical method: Bliss and Rosiello.

Observations:

- Mortality several times on day 1 and twice daily until day 14.
- Clinical signs several times on day 1 and daily until day 14.
- Body weights immediately prior to dosing and on day 9 and 15.
- Necropsy on animals that died during the study and survivors on day 15.

Results

Value: Oral LD50 = 3217 mg/kg bw for females and 3450 mg/kg bw for males; giving a combined value of 3346 mg/kg bw for both sexes

Remarks:

Dose [mg/kg bw] effect		2500		3000		3300		3500		4000		5000		DR	
Sex	Day	M	F	M	F	M	F	M	F	M	F	M	F	M	F

Clinical signs[A]	1-14	+	+	+	+	+	+	+	+	+	+	+	+	x	X
Body weight	1-15	No treatment related effects													
Necropsy[B]	15					+	+	+	+		+	+	+	x	x

Clinical observations included increased salivation, decreased activity, ptosis, prostration, laboured breathing, cold to touch, soft stool and ano-genital staining during day 1-5.

Findings consisted of foci on spleen, thymus and/or stomach, discolouration of tail, red discolouration of the stomach or lung. One female at 4000 mg/kg showed traces of autolysis.

Oral LD50 equivalent to a combined LD50 of 1044 mg/kg bw active ingredient considering the 31.2% purity of the substance.

Minor remark. The evaluation of body weight is hampered, because no control group was included in the study design.

It's not clear what the "x" mean in the DR column – suggest to delete and include in

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 24 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute oral toxicity study in rats / 715-004. 1994d

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: IRDC, Mattawan, Michigan, USA

Print File Name: 5.1.1_28088-63-3_41

Last Revised: 11-04-2005

Remarks: n/a

5.2.B ACUTE INHALATION TOXICITY

Acute inhalation toxicity data are available for CAS numbers 12068-03-0, 26447-10-9 and 28348-53-0 (32073-22-6).

5.2.C ACUTE DERMAL TOXICITY

Test Substance

CAS Number: 28088-63-3
Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA
Purity: 31.2%
Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes
Report/Study Year: 1994
Report/Study Number: 715-006
Method/Guideline Followed: US EPA TSCA 798.1100
Analytical Monitoring: n/a
Test Type: n/a
Species: Rabbit.
Strain: New Zealand White
Sex: Male/female
Vehicle: n/a
Number of Animals per Dose: 5 males and 5 females
Doses: Dermal application to the clipped skin at 2000 mg/kg bw (no vehicle; under occlusive dressing for 24 hours); no controls; feeding at fixed rate (125 g/day).
Remarks: Age: 5 months
Weight: 2.9-3.2 kg
Observations:

- Mortality several times on day 1 and twice daily until day 14.
- Clinical signs several times on day 1 and daily until day 14.
- Body weights on day 1, 8 and 15.
- Necropsy on day 15.

Results

Value: Dermal LD50 > 2000 mg/kg bw

Remarks:

Dose [mg/kg bw]effect		2000	
Sex	Day	M	F
Mortality	1-14	None	
Clinical signs(A)	1-14	+	+
Body weight	1-15	No treatment related effects	
Necropsy(B)	15	+	+

(A)Erythema with additional desquamation, observed on day 9, was observed among animals from day 3 to day 14.
(B)Findings consisted of focal or multifocal red discolouration and desqaumation of the treated skin.

Equivalent to LD50 >624 mg/kg bw active ingredient considering the 31.2% purity of the substance.

- The report indicates the treated site was covered with a 1 x 1 inch square patch. This patch is not large enough to cover the application site. Most probably this can be attributed to a typing error in the report.
- A slight body weight loss was reported during week 2. No explanation was provided. The evaluation of body weight is hampered because no control animals were included in the study design.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 22 Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute Dermal Toxicity Study in Rabbits / 715-006. 1994b

Other

Sponsor: Ruetgers-Nease Chemical, Inc

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: IRDC, Mattawan, Michigan, USA

Print File Name: 5.1.3_28088-63-3_45

Last Revised: 11-04-2005

Remarks: n/a

5.2.A SKIN IRRITATION

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA

Purity: 31.2%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: yes

Report/Study Year: 1994

Report/Study Number:	715-003
Method/Guideline Followed:	US EPA 81-5, US EPA TSCA 798.
Analytical Monitoring:	n/a
Species:	Rabbit; weight 3.3-3.6 kg
Strain:	New Zealand White
Vehicle:	n/a
Number of Animals:	3 males and 3 females
Concentration:	31% solution
Exposure:	Application of 0.5 ml test substance (no vehicle) on 2.5x2.5 cm of the clipped dorsal skin under occlusion for 4 hours.
Remarks:	Observations: Skin observations at 50 minutes, 24, 48 and 76 h after removal of the dressing using Draize method.

Results

Result:	not irritating
Primary Dermal Irritation Index (PDII):	n/a
Remarks:	No tabular data were provided in the study report as no dermal irritation observed in any animal. No mortality occurred.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 36. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Primary dermal irritation test in rabbits following a 4 hour exposure period / 715-003. 1994j

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	IRDC, Mattawan, Michigan, USA
Print File Name:	5.2.1_28088-63-3_48
Last Revised:	11-04-2005
Remarks:	n/a

5.2.B EYE IRRITATION

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt. Dimethylbenzenesulfonate CA
Purity:	31.2%

Remarks: Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP: Yes

Report/Study Year: 1994

Report/Study Number: 715-005

Method/Guideline Followed: US EPA TSCA 798.4500.

Species: Rabbit (New Zealand White), age ~4 months, weight 2.6-2.8 kg.

Vehicle: n/a

Number of Animals: 3 males and 3 females

Dose:

Value	Unit
0.1	ml

Remarks: Dosage: Application of 0.1 ml into the conjunctival sac of one eye. 31% aqueous solution.
Observations: Eye readings 1, 24, 48 and 72 hours after application using Draize method; Fluorescein staining after 72 h. The eyes of the animals remained unwashed. The substance was not applied to the other eye which served as a control.

Results

Result: Mildly irritating based on Kay & Calendra Classificaiton.

Remarks: Fluorescein staining negative.

Animal	1				2				3				4				5				6			
Effect	C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj		C	I	Conj	
Time			Red	Ch			Red	Ch			Red	Ch			Red	Ch			Red	Ch			Red	Ch
1 h *	0	1	3	2	0	1	3	2	0	1	3	2	0	1	3	3	0	1	2	2	1	0	3	2
24 h	0	0	2	1	0	0	1	1	0	0	2	1	0	1	2	1	0	0	1	1	1	0	2	1
48 h	0	0	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1	0	0	0
72 h	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

* Clear discharge and blanching was seen. C=corneal opacity I=Iris Conj=conjunctiva Red=redness Ch=chemosis

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 37. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Primary eye irritation study in rabbits / 715-005. 1994k

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	IRDC, Mattawan, Michigan, USA
Print File Name:	5.2.2_28088-63-3_50
Last Revised:	11-04-2005
Remarks:	n/a

5.2.C ACUTE DERMAL TOXICITY

Acute dermal toxicity data are available for CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

5.3.A SKIN IRRITATION/CORROSION

Skin Irritation/Corrosion data are available for CAS numbers 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.3.B EYE IRRITATION

Eye Irritation/Corrosion data are available for CAS numbers 16106-44-8, 12068-03-0, 28088-63-3, 26447-10-9, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.4 SENSITIZATION

Skin sensitization data are available for CAS numbers 12068-03-0, and 28348-53-0 (32073-22-6).

5.5 REPEATED DOSE TOXICITY

Repeated dose toxicities were measured for CAS numbers 1300-72-7 (827-21-4) and 28348-53-0 (32073-22-6).

5.6 GENETIC TOXICITY *IN VITRO*

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate Ca
Purity:	31.2%
Remarks:	Chemical name and CAS number cannot be verified from report. Noted as test article SAR 33-55. Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	yes
Report/Study Year:	1994

Report/Study Number: G94AN06.501

Method/Guideline Followed: not indicated; resembles OECD 471

Test Type: *Salmonella* plate incorporation mutagenicity assay (Ames test)

System: n/a

Test Concentration: 100, 333, 1000, 3333 and 5000 µg active ingredient/plate

Species/strain: TA98, TA100,TA1535, TA1537, TA1538

Metabolic Activation: Rat liver S9 mix (Aroclor 1254-induced).

Remarks:

Controls	Negative control: vehicle (water). Positive controls: all strains with S9, 2-aminoanthracene; TA 100 and TA1535 without S9, sodium azide; TA98 and TA1538 without S9, 2-nitrofluorene; and TA1537 without S9, 9-aminoacridine.

Results

Result: Not mutagenic with and without metabolic activation

Cytotoxic Concentration: n/a

Results:

	Test result(A)	
Tester strain	Without activation	With activation
TA98	-	-
TA100	-	-
TA1535	-	-
TA1537	-	-
TA1538	-	-

(A) +/- : positive/negative result; positive controls gave expected responses.

Remarks: n/a

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction

Flag Critical study for SIDS endpoint

Reference

Source Reference: 21. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. *Salmonella* plate incorporation mutagenicity assay (Ames test). 1994a

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Microbiological Associates Inc., Bethesda & Rockville, Maryland, USA

Print File Name:	5.5_28088-63-3_76
Last Revised:	11-04-2005
Remarks:	n/a

5.7 GENETIC TOXICITY *IN VIVO*

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, Calcium salt; Ca-dimethylbenzenesulfonate
Purity:	31.2%
Remarks:	Chemical name and CAS number cannot be verified from report. Noted as test article SAR 33-55 Substances tested are aqueous solutions; % purity equates to chemical content

Method

GLP:	Yes
Report/Study Year:	1994
Report/Study Number:	G94AN06.122
Method/Guideline Followed:	OECD Guideline 474
Test Type:	Mouse micronucleus cytogenetic assay
Species:	Mouse, 6-8 weeks old, 20-34 g.
Strain:	ICR
Sex:	Male/female
No. of animals	5 per sex per dose group per sampling time
Route of Administration:	intra-peritoneal (i.p.)
Exposure Period:	Single administration
Doses:	145, 290 and 580 mg active ingredient (a.i.)./kg bw; water controls, dosing volume 20 ml/kg bw. Dose selection was based on preliminary study with 5 animals/sex: no deaths at 200 and 500 mg a.i./kg bw, 3/10 deaths at 700 mg a.i./kg bw, 10/10 deaths at 1000 mg a.i./kg bw.
Remarks:	Statistical method: Kastenbaum-Bowman Tables. Sampling times: 24, 48 and 72 hours post-dose. Positive control: Cyclophosphamide (i.p. in water at 40 mg/kg bw) Scoring: For each animal, the following proportions were determined in bone marrow smears: • PolyChromatic Erythrocytes (PCE) in 1000 erythrocytes. • Micronucleated PolyChromatic Erythrocytes (MPCE) per 1000 PCE.

- Micronucleated NormoChromatic Erythrocytes (MNCE) per 1000 PCE.

Results

Result: Not clastogenic

Results:

Dose [mg a.i./kg bw]/effect	0	145	290	580	DR
Mortality	None				
Clinical signs(A)				+	
% PCE	no treatment related effects				
MPCE [% of PCE]	no treatment related effects				

(A) The clinical sign observed was lethargy.
Abbreviations: DR = dose related as indicated by "x", + = presence

Positive control gave the expected response.

Remarks: In males treated with 580 mg/kg that were sacrified at 72 hours, the frequency of PCEs compared to vehicle controls was decreased by 36%. This is an indication that the test substance has reached the bone-marrow and that suitable doselevels were selected.

Minor remarks The number of normochromatic erythrocytes was not reported. The proportion of MPCE was determined for 1000 PCE. This is in agreement with OECD 474 (1983); OECD 474 (1997) requires evaluation of 2000 PCE.

Data Quality

Reliability (Klimisch): 1

Remarks: Reliable without restriction, guideline study.

Flag Critical study for SIDS endpoint

Reference

Source Reference: 35. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Micronucleus cytogenetic assay in mice / SAR 33-55 (G94AN06.122). 1994i

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: Microbiological Associates Inc., Bethesda & Rockville, Maryland, USA

Print File Name: 5.6_28088-63-3_71

Last Revised: 11-04-2005

Remarks: n/a

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Test Substance

CAS Number:	28088-63-3
Identity:	Xylene sulfonic acid, calcium salt; Dimethylbenzenesulfonate CA
Purity:	31.2%
Remarks:	Chemical name and CAS number cannot be verified from report. Noted as test article SAR 33-55

Method

GLP:	Yes
Report/Study Year:	1994
Report/Study Number:	715-002
Method/Guideline Followed:	EPA TSCA, 1985
Analytical Monitoring:	From all treatment solutions prepared for week 1 and week 2 in duplicate by a gravimetric method.
Species:	Rat, age ~87 days, weight 243-312 g.
Strain:	Crl:CD
Sex:	Female
No. of animals	30 per treatment group
Route of Administration:	Gavage
Exposure Period:	daily from day 6 to 15 of gestation inclusive.
Frequency of Treatment:	Daily
Test Duration:	20 days
Doses:	150, 1500 and 3000 mg/kg bw (vehicle: water, dosing volume 10 mL/kg); solutions were prepared weekly.
Control Group:	Vehicle control
Remarks:	Statistical method: ANOVA (Bartlett, t-test, Dunnett), Chi-squared, Fisher, Kruskal-Wallis, Mann-Whitney U-test.

Analyses:

Procedures: Female rats were mated with untreated males (1/1) from the same strain. The day of observation of a copulatory plug was defined as day 0 of gestation. Mortality was checked twice daily. Clinical symptoms of dams were noted daily from day 6 to 20. Body weight and food consumption were recorded on day 0, 6, 9, 12, 16 and 20. All females were subjected to macroscopic examination on day 20 or on day of death. The uteri were removed, weighed and examined for number of corpora lutea, implantation sites and the number and location of foetuses and resorptions. Foetuses were inspected on total number, sex, weight and external, visceral (1/2 of foetuses) and skeletal (1/2 of

foetuses) defects.

Results

NOAEL Maternal: 3000 mg/kg bw/day (equivalent to 936 mg active ingredient (a.i.)/kg using 31% purity)

NOAEL Teratogenicity: 3000 mg/kg bw/day (equivalent to 936 mg a.i./kg using 31% purity)

Results: Mean measured concentration: 96-98% of nominal; stability over 10 days confirmed

Dose (mg/kg bw/day)	0	150	1500	3000	DR
Maternal data					
Mortality	0/30	0/30	1/30	0/30	
Clinical signs(A)	No treatment related effects				
Body weight /body weight gain	No treatment related effects				
Food intake □NC day 12-16				ic	
Uterus weight	No treatment related effects				
Necropsy	No treatment related effects				
Number of pregnant females	27/30	29/30	25/30	25/30	
Number of *corpora lutea* and implantation sites /dam	No treatment related effects				
Pre-implantation loss	No treatment related effects				
Post-implantation loss/ resorptions	No treatment related effects				
Embryonic / foetal resorptions	No treatment related effects				
Number of live foetuses/ dam	No treatment related effects				
Foetal data					
Number of litters included in evaluations	27	28	25	25	
Foetal weight	No treatment related effects				
External examination / sex	No treatment related effects				
Anomalies: visceral/ skeletal(B)	No treatment related effects				

(A)Focal and/or general hair loss, stained body surface, focal swelling, scabbed

and/or raised areas, laboured breathing, rales and material around the nose were observed among animals of all treatment groups. One animal of the 1500 mg/kg bw group had a subcutaneous mass.
(B)Malformations observed were incidental cases of microphthalmia (1 foetus at 150 mg/kg/day), folded retina (1 foetus in the 1500 and 3000 mg/kg/day), renal agenesis and absence of ureter (1 foetus in 150 mg/kg/day), malformed skull bones and bent scapula (1 foetus each at 150 mg/kg/day). Variations were bent tail, hydronephrosis and distended ureter. The incidence was comparable between treated and control groups.
Abbreviations: DR = dose related as indicated by "x"; ic = significant increase.

Remarks: The analytical method was based on weighing of the test substance after evaporation of the vehicle. Since the test substance was a 31.2% formulation and the additional compounds were not specified, it is not clear whether the measurements represent the test substance or both the test substance and other unknown compounds.

Single death at 1500 mg/kg/day dose associated with gavage trauma.

The increased food intake in high dose females was considered to be within ranges of biological variation.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Analyses less reliable (note 1).

Flag Critical study for SIDS endpoint

Reference

Source Reference: 32. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Developmental toxicity study in rats / 715-002. 1994g

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: IRDC, Mattawan, Michigan, USA

Print File Name: 5.8.2_28088-63-3_84

Last Revised: 11-04-2005

Remarks: It is not clear whether the concentrations should be corrected for percentage active ingredient; the results reflect a correction for 31.2% purity.

5.10 OTHER RELEVANT INFORMATION – OTHER: ANALYTICAL METHOD

Test Substance

CAS Number: 28088-63-3

Identity: Xylene sulfonic acid, calcium salt; Dimehylbenzenesulfonate CA

Purity: 31.2%

Carbon Chain Length Distribution: n/a

Remarks: n/a

Method

GLP: yes

Report/Study Year: 1994

Report/Study Number: 41658

Method/Guideline Followed: 40 CFR, Part 792.

Remarks:

Method	Column: Hypersil ODS (240 mm x 4.6 mm i.d. x 5 µ) Mobile Phase: 15% THF in ABC reagent water containing 2.5% Bu_4NOH, pH = 3.8 -4.0 with H_3PO_4 (buffer). Flow: 1.8 ml/min. Wavelength: 210 nm (UV). Injection volume 100 or 200 µl.
Procedure	HPLC Method development Two stock solutions of 0.316 and 1050 mg/l were prepared, the first in ABC, the second in hard-blended water. Initially, concentrations of 0, 0.525, 1.05, 10.5 and 1050 mg/l were prepared in duplo, however, were extended with 1.05 and 5.25 (ten replicate/tr.) mg/l since both the 0.525 and 1.05 mg/l concentrations of the first range did not have consistently acceptable recoveries and to facilitate the determination of the LOD. Calculations: percentage of peak area versus blank recovery.
Hardness	150 mg/l (as $CaCO_3$).
PH	8.3 - 8.5.
LOD	0.30 mg/l, determined as 4.65 * standard deviation of the mean measured concentration at 5.25 mg/l. However, method is not valid for concentrations below 15 mg/l.

Results

Remarks: Method can be used to determine the concentrations in water recovery for 5.25 -1050 mg/l : 101 ± 5.5%

- Percent recovery is 101% ± 5.5 and not 105% ± 5.6.
- Area percentage of 4 (first series) or 3 (second series) peaks has been taken for calculation recovery. Better should be area of highest peak only, in view of the second test-series, or the use of the 4 peaks as in the first series.
- Separate compounds of the mixture could be identified as being ortho-, meta- and para-calciumxylenesulfonate and ethylbenzenesulfonate.
- Validation below 15 mg/L is not linear.

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions. Peak area inadequate

Reference

Source Reference: 38. Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Validation of analytical methods for use in the determination of test concentrations of SAR 33-55 during aquatic toxicity studies / 41658. 1994L

Other References: n/a

Other

Sponsor: n/a

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.

Testing Laboratory: ABC Laboratories Inc., Colombia, Missouri, USA

Print File Name: 6.1_28088-63-3_24

Last Revised: 9-13-2003

Remarks: n/a

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from **http://www.epa.gov/oppt/exposure/docs/episuitedl.htm**

Mackay D., A. DiGuardo, S. Paterson and C. Cowan. 1996. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. Environmental Toxicology and Chemistry (15) 9: 1627-1637.

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Salmonella plate incorporation mutagenicity assay (Ames test). 1994a

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute Dermal Toxicity Study in Rabbits / 715-006. 1994b

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute flow-through toxicity of SAR 33-55 to Daphnia magna / 41842. 1994c

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute oral toxicity study in rats / 715-004. 1994d

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Acute toxicity of SAR 33-55 to Selenastrum capricornutum Printz / 41657, 1994e

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. CO_2 evolution test (Modified Sturm Test) with Calcium Xylenesulfonate. 1994f

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Developmental toxicity study in rats / 715-002. 1994g

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Evaluation of potential for removability: the modified semi-continuous activated sludge test with SAR 33-55 / 41655. 1994h

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Micronucleus cytogenetic assay in mice / SAR 33-55 (G94AN06.122). 1994i

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Primary dermal irritation test in rabbits following a 4 hour exposure period / 715-003. 1994j

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Primary eye irritation study in rabbits / 715-005. 1994k

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Validation of analytical methods used in the determination of test concentrations of SAR 33-55 during aquatic toxicity studies / 41658. 1994l.

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA; Acute flow-through toxicity of SAR 33-55 to rainbow trout (Oncorhynchus mykiss) / 41841, 1994m

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of the density of SS0335.01 / 41812. 1996

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of the melting temperature of SS0335.01 / 41810. 1997a

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of the octanol/water partition coefficient (Shake Flask Method) of SS0335.01 / 41814. 1997b

Ruetgers-Nease Chemical, Inc., State College, Pennsylvania, USA. Determination of water solubility (shake flask method) of SS0335.01 / 41813. 1997c

Trent University Canadian Environmental Modeling Centre at **www.trentu.ca/cemc/welcome.html**.

SIDS DOSSIER

CAS NO. 30346-73-7

xylene sulfonic acid, potassium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
12068-03-0
16106-44-8
26447-10-9
28088-63-3
28348-53-0 (32073-22-6)
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **30346-73-7**

B. Name *(IUPAC name)* **potassium xylenesulphonate**

C. Name *(OECD name)* **xylene sulfonic acid, potassium salt**

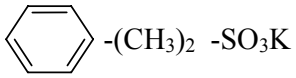
D. CAS Descriptor **Benzenesulfonic acid, dimethyl-, potassium salt**

E. EINECS-Number **250-140-3**

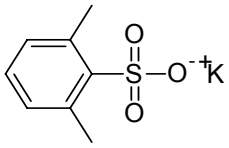
F. Molecular Formula **C8 H9 O3 S1 K1**

G. Structural Formula

Commercial xylene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the ortho, ortho isomer as a representative structure. A para-isomer would have attachments at opposite ends of the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.



.



H. Substance Group **Hydrotropes category**

I. Substance Remark

J. Molecular Weight **216 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country **Australia**

B. Lead Organization

Name of Lead Organization:

National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
Address: Team Leader, Review & Treaties, NICNAS, Australia
Tel: +61 2 8577 8880

C. Name of responder

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France

1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six "sponsored" substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ];
petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate.

1.2 SYNONYMS

xylenesulfonic acid, potassium salt
xylenesulfonate, potassium salt
potassium xylene sulfonate
benzenesulfonic acid (1-dimethyl) potassium salt
dimethylbenzenesulfonate, potassium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designated

1.7 USE PATTERN

A. General

Type of Use:	Category:
main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%
Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number:	30346-73-7
Identity:	Xylene sulfonic acid, potassium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: [K]OS(=O)(=O)c1ccc(cc1C)C MOL FOR: C8 H9 O3 S1 K1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	EPI-001
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	216.21	
Water Solubility (mg/l):	1e+006	n/a
Octanol Water Partition Coefficient (Log Kow):	-1.86	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	544.57	n/a
Melting Point (°C):	233.42	n/a
Vapor Pressure(mmHg):	1.52E-09	n/a
Henry's Law Constant (atm/(mole/m^3)):	3.123E-018	n/a
Atmospheric Oxidation Half-Life (hours):	41	n/a
Soil Adsorption Coefficient (Log Koc):	1.500	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions

Reference

Source Reference: Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Other References: n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.0.1_1300-72-7_163
Last Revised:	11-4-2005
Remarks:	n/a

2.1 MELTING POINT

Modeled melting point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Melting point was measured for CAS numbers 12068-03-0, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

2.2 BOILING POINT

Modeled boiling point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Boiling point was measured for CAS numbers 1300-72-7 and 26447-10-9.

2.3 DENSITY

Density was measured for CAS numbers 28088-63-3 and 1300-72-7 (827-21-4).

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW})

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. $\log_{10} K_{ow}$ was measured for CAS number 28088-63-3.

2.6.1 WATER SOLUBILITY & DISSOCIATION CONSTANT

Modeled water solubility is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Solubility was measured for CAS numbers 1300-72-7 (827-21-4), 12068-03-0, 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

3.0.1 EQC MODEL

Fugacity modelling has been conducted on CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	30346-73-7
Identity:	Xylene sulfonic acid, potassium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: [K]OS(=O)(=O)c1ccc(cc1C)C MOL FOR: C8 H9 O3 S1 K1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 30346737
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	1.61 E-12 cm3/molecule-sec
Half Life	80 hrs

Remarks: n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File	AOPWOO1 30346737

Name:
Last Revised: 05-09-06
Remarks: n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

Refer section 3.0.1 EQC Model.

3.4 BIODEGRADATION

Biodegradation data are available for CAS numbers 1300-72-7(827-21-4), 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6).

3.6 BIOACCUMULATION

Estimated data is available for this CAS number in EPISuite estimation of Physical/Chemical Properties in 2.0.1. Measured data is available for CAS numbers 12068-03-0 and 1300-72-7 (827-21-4).

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Fish toxicity data are available for CAS numbers 1300-72-7(827-21-4), 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2A ACUTE ORAL TOXICITY

Acute oral toxicity data are available for CAS numbers 1300-72-7(827-21-4), 12068-03-0, 16106-44-8, 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

5.2.B ACUTE INHALATION TOXICITY

Acute inhalation toxicity data are available for CAS numbers 12068-03-0, 26447-10-9 and 28348-53-0 (32073-22-6).

5.2.C ACUTE DERMAL TOXICITY

Acute dermal toxicity data are available for CAS Nos 28088-63-3 and 28348-53-0 (32073-22-6).

5.3.A SKIN IRRITATION

Skin Irritation/Corrosion data are available for CAS numbers 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.3.B EYE IRRITATION

Eye Irritation/Corrosion data are available for CAS numbers 16106-44-8, 12068-03-0, 28088-63-3, 26447-10-9, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.4 SENSITIZATION

Skin sensitization data are available for CAS numbers 12068-03-0, and 28348-53-0 (32073-22-6).

5.5 REPEATED DOSE TOXICITY

Repeated dose toxicities were measured for CAS numbers 1300-72-7 (827-21-4) and 28348-53-0 (32073-22-6).

5.6 GENETIC TOXICITY *IN VITRO*

Genetic toxicity (*in vitro*) data were collected for CAS numbers 1300-72-7 (827-21-4) and 28088-63-3, and 28348-53-0 (32073-22-6).

5.7 GENETIC TOXICITY IN VIVO

Genetic toxicity (in vivo) data were collected for CAS numbers 28088-63-3, and 28348-53-0 (32073-22-6).

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

SIDS DOSSIER

CAS NO. 16106-44-8

Toluenesulfonic acid, potassium salt

Chemical Category: Hydrotropes

Other CAS Nos. in the Category:

1300-72-7 (827-21-4)
12068-03-0
26447-10-9
28088-63-3
28348-53-0 (32073-22-6)
30346-73-7
37475-88-0

Sponsor Country: Australia
Date: June 9, 2006

1.01 SUBSTANCE INFORMATION

A. CAS number **16106-44-8**

B. Name *(IUPAC name)* **potassium toluene-4-sulphonate**

C. Name *(OECD name)* **toluene sulfonic acid, potassium salt**

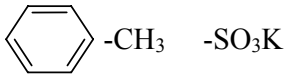
D. CAS Descriptor **Benzenesulfonic acid, 4-methyl-, potassium salt**

E. EINECS-Number **240-273-5**

F. Molecular Formula **C7 H8 O3 S1 K1**

G. Structural Formula

Commercial toluene sulfonic acid consists of mixtures of 6 isomers. The first diagram below is without isomer orientation. The second diagram depicts the ortho, ortho isomer as a representative structure. A para-isomer would have attachments at opposite ends of the benzene ring and a meta-isomer would have one open carbon between attachments on the benzene ring.



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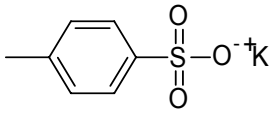

H. Substance Group **Hydrotropes category**

I. Substance Remark

J. Molecular Weight **210 grams/mole**

1.02 OECD INFORMATION

A. Sponsor Country: **Australia**

B. Lead Organization:

Name of Lead Organization:

National Industrial Chemicals Notification and Assessment Scheme (NICNAS); Australian Government Department of Health and Ageing; Australian Government Department of the Environment and Heritage (ADEH).

Contact person: Dr Sneha Satya
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C. Name of responder

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1.03 CATEGORY JUSTIFICATION

The hydrotropes category includes 10 substances as defined by 10 CAS numbers. Six of the chemical substances have High Production Volume (HPV) chemical status in one or more OECD regions. An additional four substances have also been identified as being analogues to the six “sponsored” substances and are considered part of the hydrotropes category. Two of these four substances (CAS Nos. 28088-63-3 and 16106-44-8) provide supporting data for the chemical category.

Note that two of the compounds (xylene and cumene sulfonic acid, sodium salts) have more than one CAS number. This is a result of differences in industry nomenclature practice and/or use patterns across geographical regions at the time of notification. This practice has lead to differences in how some substances are identified on national and regional chemical inventories. The structures as well as the physical/chemical and toxicologic properties of these chemical entities are essentially the same although the CAS numbers are different.

The hydrotropes category may be initially considered as three sub-groups: the methyl, dimethyl and methylethyl benzene sulfonates, (or the toluene, xylene and cumene sulfonates). Although the counter ion will also determine the physical and chemical behavior of the compounds, the chemical reactivity and classification for this purpose is not expected to be affected by the difference in counter ion (i.e., Na^+, NH_4^+, Ca^{++}, or K^+).

In general, the presence of one or two methyl groups or a methylethyl group on the benzene ring is not expected to have a significant influence on chemical reactivity. Alkyl substituents are known to be weak ortho- and para-directing activators, and the difference between methyl and methylethyl will be negligible. On going from methylbenzene (toluene) to dimethylbenzene (xylene) and to methylethylbenzene (cumene), the number of carbon atoms – and thus the organic character - increases. This will improve solubility in apolar solvents and reduce solubility in polar solvents like water. Hence, reactivity in watery solutions may differ somewhat for the hydrotropes. However, the decisive factor in determining water solubility of these compounds will be ionic character, not the number and identity of the alkyl substituents on the benzene ring.

The three sub-groups are expected to be generally comparable and predictable in their chemical behaviour (as such or in solution) and that members from one sub-group may be useful for read across to other sub-groups and to the hydrotropes category as a whole.

1.1 GENERAL SUBSTANCE INFORMATION

A. Type of Substance

element [ ]; inorganic [ ]; natural substance [ ]; organic [**X**]; organometallic [ ]; petroleum product [ ]

B. Physical State *(at 20°C and 1.013 hPa)*

gaseous [ ]; liquid [ ]; solid **[X]** for pure substance

C. Purity

The hydrotropes are ‘pure’ substances but are produced and transported in either aqueous solutions, typically at a 30-60% level of activity, or in granular solids typically at 90-95% level of activity. The other components of granular solids include sodium sulphate and water.

D. Manufacturing Process

Hydrotropes are produced by sulfonation of an aromatic hydrocarbon solvent (i.e., tolune, xylene or cumene). The resulting aromatic sulfonic acid is neutralized using an appropriate base (e.g., sodium hydroxide) to produce the sulfonate.

1.2 SYNONYMS

toluenesulfonic acid, potassium salt
toluene sulfonate, potassium salt
potassium toluene sulfonate

benzenesulfonic acid (1-methyl) potassium salt
methylbenzenesulfonate, potassium salt

1.3 IMPURITIES

Remarks: No impurities

1.4 ADDITIVES

Value: None
Remarks: No additives

1.5 QUANTITY

(a)
Value: 29,000 metric tonnes/year in the USA. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Value is consistent with the USEPA 2002 IUR (Inventory Update Rule) database.

(b)
Value: 19,000 metric tonnes/year in Europe. This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: Survey of hydrotrope manufacturers conducted by The Soap and Detergent Association in 2002. Consistent with the 2005 Human and Environmental Risk Assessment (HERA) for Hydrotropes report which addresses the laundry and cleaning uses of chemicals in Europe.

(c)
Value: 1,100 metric tonnes/year in Australia This is for all hydrotropes manufactured and/or imported; values for individual CAS numbers and substances are not available.
Source: In country use survey conducted by NICNAS.

1.6 LABELLING AND CLASSIFICATION

Labelling
Remarks: None designated

Classification
Remarks: None designate

1.7 USE PATTERN

A. General

Type of Use: **Category:**

main	Wide dispersive use
industrial	Personal and domestic use
use	Cleaning/Washing agent

Remarks:

Major uses are in personal care and household/professional cleaning products including liquid and powder laundry detergents, hand dishwashing liquid detergents, machine dishwashing rinse aids, hard surface cleaners, body washes, shampoos, hair conditioners, liquid face and hand soaps, toilet treatments, solvent hand cleaners, carpet cleaners and optical brightener products. It is estimated that 60-70% of the total tonnage is used in dishwashing liquids. There are also some relatively small volume, commercial/professional uses in liquid sulphur textile dyes, acidic recirculation cleaners, wetting agent for tanning, enzymatic recirculation cleaner for dairy and food processing, coolant system conditioner, car wash detergents, cleaners and degreasers, vinyl plastic rubber restorer, and floor strippers.

B. Uses in Consumer, Institutional and Industrial Products

Function	Amount present	Physical state
coupling agent	0.1 to 15% of formulation	powder or liquid

Remarks: Hydrotropes are used as coupling agents to solubilize water insoluble and otherwise incompatible functional ingredients.

The following table shows the percentage of hydrotropes that occurs in various types of consumer laundry/cleaning and personal care products. A blank (-) indicates the data were not available, not necessarily that those uses do not exist in those countries.

Consumer Product Type	Range of Percent Composition that is LAS		
	North America	Europe	Australia
Laundry Detergents - Powders - Liquids	 0.1-0.5% 1-10%	 up to 0.66% up to 2%	0.9–1.375%
Hard Surface Cleaners	0.1-5%	up to 6%	0.1-0.9%
Machine Dishwashing Rinse Aid	1-5%	up to 11.9%	4.1-5.5%
Hand Dishwashing Liquid Detergents	1-5%	up to 3%	1.2-5.5%
Body Washes	0.1-0.5%	-	-
Shampoo	1-5%	-	0.4-0.8%
Hair Conditioner	1-5%	-	-
Face & Hand Soaps (liquid)	10-15%	-	-
Toilet Treatments	-	up to 1.9%	0.2%
Solvent Hand Cleaner	-	-	0.8%
Carpet Cleaners	-	-	1%
Optical Brightener Product	-	-	3%

Sources:

Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables .

NICNAS for Australia uses.

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUE

Exposure limit value
Type: None established

Short term exposure limit value
Value: None established

1.9 SOURCES OF EXPOSURE

Remarks:

There is potential for workers to be exposed during manufacturing, formulation and industrial end use of products. Exposure could occur as a result of inhalation and/or dermal contact with aqueous and particulate material. The potential for human exposure to hydrotropes by inhalation is minimized by its low volatility and because most of the production, formulation and industrial end use of products are in aqueous solutions. Inhalation exposure to the solid form is likely to be minimal as dust generation is low. Dermal exposure is possible. Engineering controls (e.g., closed system operations, exhaust ventilation, dust collection) and personal protective equipment (e.g., protective clothing, eyewear, and gloves) at manufacturing and formulation facilities further mitigate worker exposure. No special engineering controls or additional personal protective equipment are uniquely specified for hydrotropes category.

Hydrotropes are used primarily in household laundry and cleaning products and in personal care products. After use, hydrotropes are discharged into the wastewater treatment system. The exposure of the general human population and of environmental organisms depends on the application of hydrotropes, the local sewage treatment practices, and on the characteristics of the receiving environment.

It is reasonable to consider that the greatest exposure to the consumer is dermal exposure following use of personal care products. The personal care products are applied as is, typically diluted during use and then rinsed off. Dermal contact does occur with personal care products and may also occur with laundry and/or cleaning products. There is some potential for incidental / accidental ingestion of, and/or eye contact with, product during handling and use. Low volatility minimizes the potential for inhalation.

Sources:

The Soap and Detergent Association 2002 Survey of production, use and exposure information provided by the member companies of the Hydrotropes Consortium and the SDA HPV Task Force.

The Soap and Detergent Association 2002 Habit and Practice Survey.

AISE/HERA 2002. HERA Task Forces Human Habits and Uses Tables.

NICNAS for Australia uses.

1.10 ADDITIONAL REMARKS

A. Options for Disposal

Remarks: Unused hydrotropes may be recovered for reprocessing or disposed of by incineration or by flushing to sewage system; used material enters sewage system and is treated at WWTP. Spills may be recovered for reprocessing or disposal.

B. Last Literature Search

Remarks:

2002/2003. Including survey of Hydrotrope Consortium member companies for quantity, uses, and unpublished studies on physical/chemical properties, environmental fate, environmental effects and mammalian toxicity. Also literature searches were conducted employing a strategy utilizing databases available from the U.S. Chemical Information Systems and the European International Uniform Chemical Information Database (IUCLID) and Institute for Systems, Informatics and Safety (ISIS) Environmental Chemicals Data Information Network (ECDIN) databases.

2.0.1 EPISUITE™ ESTIMATION OF PHYSICAL/CHEMICAL PROPERTIES

Test Substance

CAS Number:	16106-44-8
Identity:	Toluene sulfonic acid, potassium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: c1cc(C)ccc1S(=O)(=O)OK MOL FOR: C7 H7 O3 S1 K1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	EPI-001
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate	Exp. database Match
Molecular Weight (grams/mole):	210.29	
Water Solubility (mg/l):	1e+006	n/a
Octanol Water Partition Coefficient (Log Kow):	-2.40	n/a
Bioconcentration Factor (Log BCF):	0.500	
Boiling Point (°C):	532.98	n/a
Melting Point (°C):	228.00	n/a
Vapor Pressure(mmHg):	2.63E-011	n/a
Henry's Law Constant (atm/(mole/m^3)):	7.277E-018	n/a
Atmospheric Oxidation Half-Life (hours):	105	n/a
Soil Adsorption Coefficient (Log Koc):	1.282	

Remarks: n/a

Data Quality

Reliability (Klimisch): 2

Remarks: Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File Name:	2.0.1_16106-44-8_167
Last Revised:	11-04-2005
Remarks:	n/a

2.1 MELTING POINT

Modeled melting point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Melting point was measured for CAS numbers 12068-03-0, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

2.2 BOILING POINT

Modeled boiling point is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Boiling point was measured for CAS numbers 1300-72-7 and 26447-10-9.

2.3 DENSITY

Density was measured for CAS numbers 28088-63-3 and 1300-72-7 (827-21-4).

2.4 VAPOUR PRESSURE

Modeled vapour pressure is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Vapour pressure was measured for CAS number 1300-72-7.

2.5 PARTITION COEFFICIENT (LOG_{10} K_{OW})

Modeled partition coefficient is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. $\log_{10} K_{ow}$ was measured for CAS number 28088-63-3.

2.6.1 WATER SOLUBILITY & DISSOCIATION CONSTANT

Modeled water solubility is provided for this chemical in 2.0.1 EPISuite™ estimation of Physical/Chemical Properties. Solubility was measured for CAS numbers 1300-72-7 (827-21-4), 12068-03-0, 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

3.0.1 EQC MODEL

Fugacity modelling has been conducted on CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

3.1.A PHOTODEGRADATION

Test Substance

CAS Number:	16106-44-8
Identity:	Toluene sulfonic acid, potassium salt
Purity:	n/a
Carbon Chain Length Distribution:	n/a
Remarks:	SMILES: c1cc(C)ccc1S(=O)(=O)OK MOL FOR: C7 H7 O3 S1 K1

Method

GLP:	n/a
Report/Study Year:	n/a
Report/Study Number:	AOPWOO1 16106448
Method/Guideline Followed:	n/a
Remarks:	n/a

Results

	Estimate
Overall Rate Constant	1.22 E-12 cm3/molecule-sec
Half Life	105 hrs
Remarks:	n/a

Data Quality

Reliability (Klimisch):	2
Remarks:	Reliable with restrictions

Reference

Source Reference:	Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm
Other References:	n/a

Other

Sponsor:	n/a
Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Testing Laboratory:	n/a
Print File	AOPWOO1 16106448

Name:
Last Revised: 05-09-06
Remarks: n/a

3.1.B STABILITY IN WATER

No measured data are available for hydrolysis of the hydrotropes category, and the chemicals cannot be modeled in EPIWIN; however, since commercial products are available in aqueous solutions and these products are stable, the lack of hydrolysis data is not considered a significant deficiency. The salts are expected to dissociate completely in water and hydrotropes are known to be readily biodegradable.

3.3 TRANSPORT AND DISTRIBUTION

Refer section 3.0.1 EQC Model.

3.4 BIODEGRADATION

Biodegradation data are available for CAS numbers 1300-72-7(827-21-4), 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6).

3.6 BIOACCUMULATION

Estimated data is available for this CAS number in EPISuite estimation of Physical/Chemical Properties in 2.0.1. Measured data is available for CAS numbers 12068-03-0 and 1300-72-7 (827-21-4).

4.1 FISH TOXICITY (ACUTE AND PROLONGED)

Fish toxicity data are available for CAS numbers 1300-72-7(827-21-4), 26447-10-9, 28088-63-3, and 28348-53-0 (32073-22-6).

4.2 AQUATIC INVERTEBRATES TOXICITY (ACUTE AND PROLONGED)

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Aquatic invertebrates toxicity data are available for CAS numbers 1300-72-7(827-21-4), 28088-63-3, and 28348-53-0 (32073-22-6).

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

Microorganisms toxicity data are available for CAS number 28348-53-0.

5.2.A ACUTE ORAL TOXICITY

Test Substance

CAS Number: 16106-44-8
Identity: Toluene sulfonic acid, potassium salt
Purity: not indicated
Remarks: 50% aqueous concentration

Method

GLP: n/a
Report/Study Year: 1978
Report/Study Number: SDAHT07
Method/Guideline Followed: not indicated
Test type: n/a
Species: Rat
Remarks: No details provided

Results

Value: LD50 = 4400 mg/kg
Remarks: 95% confidence interval of 3800 – 5000 mg/kg

Data Quality

Reliability (Klimisch): 4
Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50 The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency: Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name: 5.1.1_16106-44-8_120
Last Revised: 6-22-2004
Remarks: n/a

5.2.B ACUTE INHALATION TOXICITY

Acute inhalation toxicity data are available for CAS numbers 12068-03-0, 26447-10-9 and 28348-53-0 (32073-22-6).

5.2.C ACUTE DERMAL TOXICITY

Acute dermal toxicity data are available for CAS numbers 28088-63-3 and 28348-53-0 (32073-22-6).

5.3.A SKIN IRRITATION

Skin Irritation/Corrosion data are available for CAS numbers 12068-03-0, 26447-10-9, 28088-63-3, 28348-53-0 (32073-22-6), and 1300-72-7 (827-21-4).

5.3.B EYE IRRITATION

Test Substance

CAS Number:	16106-44-8
Identity:	Toluene sulfonic acid, potassium salt
Purity:	Not indicated
Remarks:	n/a

Method

GLP:	n/a
Report/Study Year:	1978
Report/Study Number:	SDAHT07
Method/Guideline Followed:	not indicated
Species:	Rabbit
Vehicle:	n/a
Number of Animals:	6
Dose:	n/a
Remarks:	20% solution undiluted; non-rinsed and rinsed 50% solution rinsed

Results

Result: Irritating

Remarks: Non-rinsed showed irritation with recovery of two animals in 1 hour and one animal in 7 hours. Rinsed showed slight irritation with recovery in a few hours.
With 50% solution rinsed slight irritation was observed.

Data Quality

Reliability (Klimisch): 4

Remarks: Not assignable. Secondary literature.

Reference

Source Reference: 50. The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978

Other

Submitting Agency:	Hydrotrope Consortium, K. Stanton, kstanton@sdahq.org, The Soap and Detergent Association, 1500 K St. NW, Suite 300, Washington, DC 20005.
Print File Name:	5.2.2_16106-44-8_128
Last Revised:	6-22-2004
Remarks:	n/a

5.4 SENSITIZATION

Skin sensitisation data are available for CAS numbers 12068-03-0, and 28348-53-0 (32073-22-6).

5.5 REPEATED DOSE TOXICITY

Repeated dose toxicities were measured for CAS numbers 1300-72-7 (827-21-4) and 28348-53-0 (32073-22-6).

5.6 GENETIC TOXICITY *IN VITRO*

Genetic toxicity (*in vitro*) data were collected for CAS numbers 1300-72-7 (827-21-4) and 28088-63-3, and 28348-53-0 (32073-22-6).

5.7 GENETIC TOXICITY IN VIVO

Genetic toxicity (in vivo) data were collected for CAS numbers 28088-63-3, and 28348-53-0 (32073-22-6).

5.8 CARCINOGENICITY

Carcinogenity data were collected for CAS number 1300-72-7 (827-21-4).

5.9.B REPRODUCTIVE TOXICITY – DEVELOPMENTAL TOXICITY

Reproductive toxicity (developmental) data were collected for CAS number 28088-63-3.

Epiwin v. 3.11 Chemical Property Estimation Software, US EPA (2003), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

Epiwin v. 3.12 Chemical Property Estimation Software, US EPA (2005), programs can be downloaded from http://www.epa.gov/oppt/exposure/docs/episuitedl.htm

The Soap and Detergent Association, Washington, DC, USA. Summary of human and environmental safety data on hydrotropes. 1973 - 1978