FOREWORD INTRODUCTION

Benzene, C10-C16 alkyl derivatives

(123-01-3, 6742-54-7, 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 12813-60-1)

SIDS Initial Assessment Report

for SIAM 3

(Williamsburg, USA, 13-15 February 1995)

Chemical Name: Dodecylbenzene and undecylbenzene (isomers Benzenes, C_{10}-C_{16} alkyl derivatives)

CAS No: 123-01-3 and 6742-54-7 (68648-87-3,129813-58-7, 68442-69-3, 129813-59-8, 129813-60-1)

Sponsor Country: United States

National SIDS Contact Point in Sponsor Country:

Oscar Hernandez, Director RAD (7403M)
U.S. Environmental Protection Agency
1200 Pennsylvania Ave, Washington, DC 20460
Tel : 202 564-7641
Fax : 202 564-7430
E-mail hernandez.oscar@epa.gov

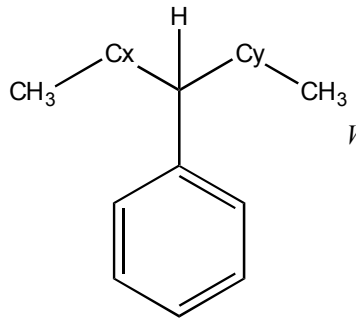
History: This chemical was assigned to the United States and first discussed at SIAM 3. At the meeting, it was agreed that no further testing was needed. In addition, further information can be obtained from the EU risk assessment completed in 1997.

Test: no testing (x)
testing (_)

Comments: The information in the report refers to various mixtures of linear alkylbenzenes, which may contain dodecylbenzene (123-01-3) and undecylbenzene (6742-54-7). Manufacturers do not produce dodecylbenzene and undecylbenzene in significant commercial quantity as pure materials. Instead, they produce various mixtures of long-chain linear alkylbenzenes with the alkyl group containing from 10 to 16 carbon atoms.

Date of Circulation:
Revised: May 2002

SIDS INITIAL ASSESSMENT PROFILE

CAS No.	123-01-3 and 6742-54-7
Chemical Name	Benzene, C10-C16 Alkyl derivatives
Structural Formula	 *Where x + y = 7 - 13* and x = 0 - 6

CONCLUSIONS AND RECOMMENDATIONS

This group of chemicals is currently of low priority for further work.

SHORT SUMMARY WHICH SUPPORTS THE REASONS FOR THE CONCLUSIONS AND RECOMMENDATIONS

Attention: This chemical is to be discussed with 6742-54-7, 68442-69-3, 68648-87-3, 129813-58-7, 129813-59-8 and 129813-60-1 as a group of Alkylbenzenes.

Dodecylbenzene (123-01-3) and undecylbenzene (6742-54-7) are not produced in significant commercial quantity as pure materials. Manufacturers produce various mixtures of long-chain linear alkybenzenes with the alkyl group containing from 10 to 16 carbon atoms.

The production of linear alkylbenzene sulfonate (LAS), a detergent surfactant, consumes greater that 98% of all linear alkylbenzenes. The potential for employee exposure is limited and infrequent. The low vapor pressure and controls utilized for other materials used in the process limits the emission of liner alkylbenzenes to air.

Linear alkylbenzenes undergo rapid primary biodegradation in natural waters and complete mineralization by microorganisms under aerobic conditions and in sludge amended soils. Due to their metabolism, these materials possess little potential to bioconcentrate in fish. They do not appear to undergo direct photolysis or chemical change in the environment.

Linear alkylbenzene, at various concentrations up to and exceeding their approximate water solubility limits, had no acute effects on all the species tested, except *Daphnia magna*. Linear alkylbenzene is 10 times more toxic to Daphnids than fish in acute tests.

Linear alkylbenzenes are not acutely toxic. Data from repeat exposure, reproductive and genotoxicity studies also indicate a low potential for toxic effects.

The levels of both consumer and occupational exposure are expected to be very low based on their physical and chemical properties, use and handling patterns.

NATURE OF FURTHER WORK RECOMMENDED

No need for further work.

FULL SIDS SUMMARY

CAS NO: 123-01-3 and 6742-54-7		SPECIES	PROTOCOL	RESULTS
PHYSICAL-CHEMICAL				
2.1	Melting Point	--	--	< -45.5°C
2.2	Boiling Point	--	ASTM D-86	251-320°C (various blends)
2.3	Density	--	--	NA
2.4	Vapour Pressure	--	--	6.5 x 10^{-5} kPa at 25°C (4.87 x 10^{-4}mmHg)
2.5	Partition Coefficient (Log K_{ow})	--	Calculated	5.72-5.75 at 27°C
2.6 A.	Water Solubility	--	GC	0.041 mg/L at 25°C
B.	pH	--	--	NA
	pKa	--	--	NA
2.12	Oxidation: Reduction Potential	--	--	NA
	Henry's Law Constant		Measured	7.1 x 10^{2} torr-L/mole (9.34 x 10^{-4} atm-m^3/mol)
ENVIRONMENTAL FATE AND PATHWAY				
3.1.1	Photodegradation	--	Measured/ EPA/TSCA	<1% photodegradation in water after 14 days (Alkylate 215)
3.1.2	Stability in Water	--	Measured	Half-life 4-9 days (Alkylate 225)
3.2	Monitoring Data	--	Measured	≤ 1.0 ug/L in water downstream from sewage treatment plants
				≤ 0.87 mg/kg in sediments downstream from sewage treatment plants
3.3	Transport and Distribution	--	Estimated/EPI WIN Level III fugacity model	Air = 3.9%, Water = 38.4%, Soil = 54.4, Sediment = 3.3%
3.5	Biodegradation		Measured/ EPA	56-61% degradation (% CO_2, theoretical)
3.7	Bioaccumulation	Lepomis macrochirus	Measured/ ASTM	BCF = 35
ECOTOXICOLOGY				
4.1	Acute/Prolonged Toxicity to Fish	Salmo gairdneri	24-96 hr/ EPA	LC50 > water sol. (Alkylate 215)
		Pimephales promelas	24-96 hr/EPA	LC50 > water sol. (Alkylate 215, 225, 230)
		Lepomis macrochirus	24-96 hr/EPA	LC50 > water sol. (Alkylate 215)
4.2	Acute Toxicity to Aquatic Invertebrates	Daphnia magna	48 hr/EPA	EC50 = 0.08 mg/L (Alkylate 215)
			48 hr/EPA	EC50 = 0.009 mg/L (Alkylate 225)
			48 hr/EPA	EC50 = 0.01 mg/L (Alkylate 230)
			48-hr/ECC	NOEC > water sol. (C_{10}-C_{13} LAB)
			48 hr/ECC	NOEC > 0.04 mg/L (C_{10}-C_{13} LAB)
			48 hr /OECD 202, part 1	NOEC > 0.1 mg/L (C_{10}, C_{12}, C_{14} LAB)

CAS NO: 123-01-3 and 6742-54-7		SPECIES	PROTOCOL	RESULTS
		Mysidopsis bahia	96 hr/ASTM	LC50 > water sol. (Alkylate 215)
		Gammarus fasciatus		No toxicity up to water sol.(Alkylate 215)
		Paratanytarsus parthenogenetica	48 hr/EPA	LC50 > water sol. (Alkylate 215)
		Chironomus tentans	96 hr/ASTM	LC50 > water sol. (Alkylate 225)
4.3	Toxicity to Aquatic Plants e.g. Algae	Selenastrum capricornutum	96-hr/ Printz assay	EC50 > water sol. (Alkylate 215)
		Scenedesmus subspicatus	72 hr/OECD TG 201	NOEC = 0.05 mg/L (above water sol.) (Euro. Com. LAB, C_{10}-C_{13})
4.4	Toxicity to Microorganisms			No data
4.5.1	Chronic Toxicity to Fish	Brachydanio rerio	84/449/EEC OECD TG 203	NOEC > water sol.(C_{10}-C_{13} LAB) NOEC > 57.8 µg/L (C_{10}-C_{13} LAB)
4.5.2	Chronic Toxicity to Aquatic Invertebrates (*Daphnia*)	Daphnia magna	21 days/ EPA/ASTM	MATC = 0.0075 mg/L (Alkylate 215) MATC = 0.013 mg/L (Alkylate 230)
		Chironomus tentans	14 days	MATC > 0.125 mg/L (Alkylate 225)
4.6.1	Toxicity to Soil Dwelling Organisms	--	--	No data
4.6.2	Toxicity to Terrestrial Plants	--	--	No data
4.6.3	Toxicity to Other Non-Mammalian Terrestrial Species (Including Birds)	--	--	No data
TOXICOLOGY				
5.1.1	Acute Oral Toxicity	Rat	Acute lethality	LD50 = 17,000 mg/kg (Alkylate 215)
		Rat	Acute lethality	LD50 = 28,200 mg/kg (Alkylate 225)
		Rat	Acute lethality	LD50 = 20,800 mg/kg (Alkylate 230)
		Rat	Acute lethality	LD50 = >34,080 mg/kg (Nalkylene 500)
		Rat	Acute lethality	LD50 = >35,800 mg/kg (Nalkylene 600)
		Rat	Acute lethality	LD50 = >5,000 mg/kg (Nalkylene 600L)
		Rat	Acute lethality	LD50 = >5,000 mg/kg (Nalkylene 550L)
5.1.2	Acute Inhalation Toxicity	Rat	Acute lethality	LC50 > 1.82 mg/L (Alkylate 215)
		Rat	Acute lethality	LC50 = 71 mg/L (nom.) (Nalkylene 500)
5.1.3	Acute Dermal Toxicity	Rabbit	Acute lethality	LD50 = >10,200 mg/kg (Alkylate 215)
		Rabbit	Acute lethality	LD50 = >10,200 mg/kg (Alkylate 225)
		Rabbit	Acute lethality	LD50 = >10,200 mg/kg (Alkylate 230)
		Rabbit	Acute lethality	LD50 = ~2,000 mg/kg (Nalkylene 500)
		Rabbit	Acute lethality	LD50 = >5,000 mg/kg (Nalkylene 500)
		Rabbit	Acute lethality	LD50 = >2,000 mg/kg (Nalkylene 600L)

CAS NO: 123-01-3 and 6742-54-7		SPECIES	PROTOCOL	RESULTS
		Rabbit	Acute lethality	LD50 = >2,000 mg/kg (Nalkylene 550L)
5.2.1	Skin Irritation	Rabbit	Draize (72 hr)	3.8/8.0; mod. irritating. (Alkylate 215)
		Rabbit	Draize (24 hr)	3.6/8.0; mod. irritating (Alkylate 225)
		Rabbit	Draize (24 hr)	3.0; slight. irritating (Alkylate 230)
		Rabbit	Draize (48 hr)	3.6 (Nalkylene 500)
		Rabbit	Draize (24 hr)	4.6 (Nalkylene 500)
		Rabbit	Draize (24 hr)	2.5 (Nalkylene 600L)
		Rabbit	Draize (24 hr)	2.4 (Nalkylene 600)
		Rabbit	Draize (24 hr)	3.6 (Nalkylene 550L)
		Human	0.2 mL, undiluted	Primary irritant in 149/205 individuals (Alkylate 215)
5.2.2	Eye Irritation	Rabbit	Draize (1 hr)	20.8/110; slight. irritating. (Alkylate 215)
		Rabbit	Draize (1 hr)	14.4/110; slight. irritating (Alkylate 225)
		Rabbit	Draize (1 hr)	11.8/110; slight. irritating (Alkylate 230)
		Rabbit	Draize (1 hr)	2.0; non-irritating (Nalkylene 500)
		Rabbit	Draize (24 hr)	0.7; non-irritating (Nalkylene 600L)
		Rabbit	Draize (3 hr)	5.3; non-irritating (Nalkylene 600)
		Rabbit	Draize	0; non-irritating (Nalkylene 550L)
5.3	Skin Sensitization	Human	NG	0 of 205 sensitized (Alkylate 215)
		Guinea pig	OECD TG 406	0 of 20 sensitized (C_{10}-C_{13} LAB)
5.4	Repeated Dose Toxicity	Rat	4-wk; inhal./ EPA/TSCA	NOAEL = 100 mg/m^3 (Alkylate 215)
			14 wk; inhal./ EPA/TSCA	NOAEL = 102 mg/m^3 (Alkylate 215)
			4 wk, dietary/ EPA/TSCA	NOAEL < 2500 ppm (Alkylate 215)
			4 wk, inhal./ EPA/TSCA	NOAEL = 29 mg/m^3 (Alkylate 225)
			4 wk; inhal./ EPA/TSCA	NOAEL < 32 mg/m^3 (Alkylate 230)
5.5	Genetic Toxicity In Vitro			
A.	Bacterial Test (Gene mutation)	Salmonella typhimurium	Ames test/ EPA/TSCA	Negative with and without activation (Alkylate 215)
		Salmonella typhimurium	Ames test/ EPA/TSCA	Negative with and without activation (Alkylate 225)
		Salmonella typhimurium	Ames test/ EPA/TSCA	Negative with and without activation (Alkylate 230)
B.	Non-Bacterial In Vitro Test	Chinese hamster ovary cells	Cytogenetic/ EPA/TSCA	Negative with and without activation (Alkylate 215)
		Chinese hamster ovary cells	Cytogenetic/ EPA/TSCA	Negative with and without activation (Alkylate 225)
		Chinese hamster ovary cells	Cytogenetic/ EPA/TSCA	Negative with and without activation (Alkylate 230)
5.6	Genetic Toxicity In Vivo	Rat, bone marrow	Chromosome aberration/ EPA/TSCA	Negative (Alkylate 215)
		Rat, bone	Chromosome	Negative (Alkylate 225)

CAS NO: 123-01-3 and 6742-54-7		SPECIES	PROTOCOL	RESULTS
		marrow	aberration/ EPA/TSCA	
		Rat, bone marrow	Chromosome aberration/ EPA/TSCA	Negative (Alkylate 230)
5.7	Carcinogenicity	Mice	18 month skin painting study	Enhanced mortality and severe skin irritation effects (hyperplasia and pigment leakage); negative for complete carcinogenesis, but promoting effect reported (C12-C20 monosubstituted LAB)
5.8	Toxicity to Reproduction	Rat	Two-generation/oral Other EPA/TSCA	NOEL = 50 mg/kg (P generation) NOEL = 5 mg/kg (F1 generation) NOEL = 5 mg/kg (F2 generation) (Alkylate 215)
5.9	Developmental Toxicity/ Teratogenicity	Rat	GD 6-15/oral Other: EPA/TSCA	NOEL = 125 mg/kg maternal toxicity NOEL = 125 mg/kg embryotoxicity (Alkylate 215)
		Rat	GD 6-15/oral Other: EPA/TSCA	NOEL = 125 mg/kg maternal toxicity NOEL = 125 mg/kg embryotoxicity (Alkylate 230)
5.11	Experience with Human Exposure	Human		No data

SIDS INITIAL ASSESSMENT REPORT (SIAR)

Benzene, C_{10}-C_{16} Alkyl derivatives

CAS No. 123013 and 6742547; (isomers 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 129813-60-1)

1. IDENTITY

Commercially available LAB is a mixture of substances composed of a benzene ring attached to a single chain of carbon atoms. Various isomers are possible since the benzene ring may be positioned at all carbons of the alkyl chain except the terminal carbon. The number of carbons per alkyl chain ranges for any given product from ten to sixteen. The CAS registry numbers used by U.S. manufacturers of these materials are: 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 129813-60-1.

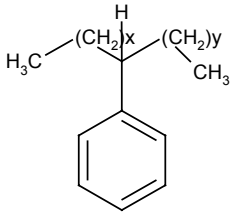
Name : Benzene, C_{10}-C_{16} Alkyl derivatives

Synonyms: Linear alkylbenzenes; LAB; Alkylate 215; Alkylate 225; Alkylate 229; Alkylate 230; Nalkylene 550L; Nalkylene 600L; Nalkylene 500; Nalkylene 500L; Nalkylene 580L, Nalkylene 600; Nalkylene 575L, Detergent Alkylate, and Alkylate

CAS Numbers: 123-01-3 (dodecylbenzene); 6742-54-7 (undecylbenzene); NOTE: CAS Nos. for mixtures used by manufacturers are: 68648-87-3; 129813-58-7; 68442-69-3; 129813-59-8; and 129813-60-1.

Molecular Formula : C_6H_5 C_nH_{2n+1} (n = 10-16)

Structural Formula :



Where x + y = 7- 13 and x = 0-6

Physical State: liquid

Degree of Purity : Linear alkylbenzene mixtures are typically 87- 94% pure.

Major Impurity : Impurities include dialkyltetralins and isoalkylbenzenes.

Essential Additives : Not applicable

Physical-chemical properties

Melting Point:	<45.5°C	Vista, 1991
Boiling Point:		
Alkylate 215 (<1%C_9, 16%C_{10}, 43% C_{11}, 40%C_{12}, 1%C_{13}, <1%C_{14})	279-295°C (101 kPa)	Monsanto, unpub.
Alkylate 225 (<1%C_9, 7%C_{10}, 25%C_{11}, 48%C_{12}, 19%C_{13}, 1%C_{14})	277-309°C (101 kPa)	Monsanto, unpub.
N-600L (<1%C_9, <1%C_{10}, 1%C_{11}, 23%C_{12}, 50%C_{13}, 25%C_{14}, <1%C_{15})	279-292°C (101 kPa)	Dixie Services, 1991
N-500 (1%C_9, 21%C_{10}, 39%C_{11}, 31%C_{12}, 7%C_{13}, <1%C_{14})	279-292°C (101 kPa)	Dixie Services, 1991
Alkylate 229 (<1%C_9, 1.1%C_{10}, 7.6% C_{11}, 36.4%C_{12}, 45.2%C_{13}, 9.6% C_{14}, <1%.C_{15})	289-307°C (101 kPa)	Huntsman, unpub.
Alkylate 230 (1%C_{10}, 2% C_{11}, 16%C_{12}, 50%C_{13}, 30%C_{14}, 1% C_{15})	251-320°C (101 kPa)	Huntsman, unpub.
Vapour Pressure:		
Alkylate 215 (<1%C_9, 16%C_{10}, 43%C_{11}, 40%C_{12}, 1%C_{13}, <1%C_{14})	6.5×10^{-5} kPa (25°C) (4.87×10^{-4} mmHg)	Monsanto Rept, ABC 27561
Water Solubility:	0.041 mg/L (25°C)	Monsanto Rept, ABC 27560
Partition Coefficient (Log P_{OW}):	5.72-5.75 (27°C, calc.)	Gledhill et al., 1991
Flash Point:	135- 137 °C	Monsanto, unpub.
Henry's Law Constant	9.34×10^{-4} atm-m^3/mol	Monsanto, ES-81-SS-41

2. GENERAL INFORMATION ON EXPOSURE

Greater than 98% of all LAB is used as an intermediate in the production of linear alkylbenzene sulfonate (LAS), a detergent surfactant. LAS is used in light-duty liquid dishwashing compounds, heavy-duty liquid and powder laundry detergents, all-purpose cleaners and industrial cleaners. Consumers may be exposed to small amounts of residual LAB in the LAS contained in these products. LAB also finds minor use in the paper, flooring and functional fluid industries.

The potential for employee exposure is limited and infrequent. The low vapor pressure of LAB and the controls used in its manufacture limit its emission to air. Any wastes or spills generated during manufacture are collected and incinerated or placed in landfills.

2.1 Environmental Exposure and Fate

2.1.1 Environmental Exposure

Detergent manufacture and non-detergent-related usage releases minor amounts of linear alkylbenzene to water. The low vapor pressure of linear alkylbenzene [6.5 x 10^{-5} kPa at 25°C for Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}), Monsanto Report ABC 27561] suggests minimal environmental entry to the air from holding tanks and spray drying of powdered detergents. Use of improved tower scrubbers assures that potential spray drying release is small. Aqueous solubility (0.041 mg/l at 25°C; Monsanto Report ABC 27560), vapor pressure (6.5 x 10^{-5} kPa at 25°C; Monsanto Report ABC-27561), and soil partitioning measurements (2.2 x 10^4; Monsanto Study ES-81-SS-41) indicate that linear alkylbenzenes are distributed in the air and adsorbed to soil or sediment.

LAB levels have been measured in receiving waters and sediments around selected U.S. municipal wastewater treatment plants. The specific plants studied were chosen because they were situated on small streams that provided low dilution of plant effluents. Concentrations ranged from non-detectable to 1 µg/L and non-detectable to 0.87 mg/kg for receiving waters and sediments, respectively (Gledhill et al., 1991)).

2.1.2 Environmental Fate

Using EPIWIN model version 3.10, level III fugacity modeling was performed (U.S. EPA, 2002). Model results estimated, that when equal distribution is assumed, the linear alkylbenzenes would distribute in the general environment in the following pattern:

Compartment	Percent Distribution
Air	3.9
Water	38.4
Soil	54.4
Sediment	3.3

It should be noted, that when using the EPIWIN model version 3.10 and entering the CAS number 123-01-3, the corresponding structure has the benzene ring on the terminal carbon which is inconsistent with the actual structure as defined in section 1 of the SIAR (the benzene ring is located on any carbon besides the terminal carbon.) As a result, the CAS number input is not valid when using EPIWIN and the structure was input manually with the benzene ring being located on the third carbon. The parameters used in the fugacity model were as follows: mol. wt. = 246.44 in the range of all the LABs; Henry's Law Constant = 9.34 x 10^{-4} atm-m^3/mole, Log K_{ow} = 5.7 and a Soil K_{oc} = 22,000, WS = 0.041 mg/L, BP = 279^{0}C (median range of LABs); MP = –45^{0}C; $t_{1/2}$ values (air) = 6.4 hrs, (water) = 96 hrs, (soil) = 96 hrs and (sediment) = 384 hrs; default emission values of 1000 kg/hr were assumed for air, water, and soil with 0 for sediment.

Photodegradation

Linear alkylbenzenes do not appear to undergo direct photolysis or chemical change in the environment. Less than 1% degradation occurred when acetonitrile solutions of Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) were exposed to direct sunlight for 14 days (Gledhill et al., 1991).

Biodegradation

Linear alkylbenzenes undergo rapid primary and complete biodegradation in natural waters. The average half-life in waters for commercial range LAB was 4.1 days (Gledhill et al., 1991). Microorganisms in sewage sludge, soil and sludge amended soil rapidly and completely biodegrade LAB. This has been confirmed with a [^{14}C] -benzene ring labeled model LAB compound. The average half lives for the conversion of LAB to CO_2 were: activated sludge- 2.6 hours, soil- 3.2 to 4.5 days, and sludge amended soil- 15 to 33 days (Holt, 1992; Holt and Berstein, 1992). The aerobic biochemical pathway for the biodegradation of LAB is shown in Appendix 1. This pathway is based on the similarity of the aerobic pathways for LAB and its sulfonate, LAS, except desulfonation is not required for the complete mineralization of LAB (Bayona et al., 1986).

The anaerobic biodegradation of short chain alkylbenzenes such as toluene, xylene and ethylbenzene has been shown (Zeyer et al., 1986; Grvbic and Vogel, 1987; Wilson et al., 1986; Major et al., 1988; Kuhn et al., 1988; Cozzarelli et al., 1990). Clearly the anaerobic biodegradation of commercial range LAB occurs but at a slow rate (Takada and Ishiwatari, 1990). Data from southern California, the western Mediterranean and to lesser extent, Tokyo Bay, show that LAB biodegrades and is not accumulating in coastal sediments (Eganhouse et al., 1983; Valls et al., 1989; Takada et al., 1992). It is also reasonable to assume that dialkytetralins and isoalkylbenzenes are biodegradable since the closely related chemical, tetralin, is biodegradable (Schreiber and Winkler, 1983; Sikkema and de Bont, 1991) and the sulfonated forms of dialkytetralins and isoalkylbenzenes are also completely biodegradable (Nielsen et al., 1997; Cavalli et al., 1996a; Cavalli et al., 1996b).

Sewage treatment plants remove most of the LAB that is released in sewage. Average percent removals range from 69% to >98% for trickling filter and activated sludge plants, respectively (Gledhill et al., 1991).

Bioaccumulation

LAB possesses little potential to bioconcentrate in fish due to its rapid metabolism. Measured bioconcentration factors in fish range from 35 to 444 versus predicted values ranging from 6,300 to 3,500,000 (Werner and Kimerle, 1982; Burke et al., 1991).

2.2 Human Exposure

2.2.1 Occupational exposure

LAB is manufactured and processed in systems that reduce direct contact with workers. Gloves and other protective equipment are typically used when handling LAB or process equipment. Incidental exposure to LAB may occur during routine manufacturing activities that include: 1) sampling and equipment decontamination; 2) rail car or truck loading and unloading; and 3) sample analysis, draining process vessels, including manipulating valves and measuring tank levels, pump repair and general maintenance. Estimated frequencies and durations per worker for such activities are as follows: 1) sampling, 0.25-1 hour/day for 10-100 days/year, 2) loading/unloading, 1-8 hours/day for 100-250 days/year; and 3) sample analysis, etc., 1-8 hours/day for 100-250 days/year (Radian Corp. and Versar, Inc., 1995).

Laboratory studies show that repeated exposure to LAB may be irritating to the skin. Material Safety Data Sheets provide skin hazard warnings and recommendations for protective clothing for use during handling that reduces the potential for skin exposure. Significant dermatitis among workers handling LAB has not been reported.

The low vapor pressure of LAB limits exposure by the inhalation route. Estimated annual air releases of LAB from three manufacturing facilities in the U.S. are 45 kg/yr for fugitive emissions and 910 kg/yr for stack releases (Radian Corp. and Versar, Inc., 1995). Using conservative atmospheric dispersion models (USEPA, 1994), estimated environmental concentrations from these releases are 2.2×10^{-4} and 8.9×10^{-4} mg/m^3, respectively (Radian Corp. and Versar, Inc., 1995).

2.2.2 Public Exposure

Detergent manufacturers sulfonate LAB to produce linear alkylbenzene sulfonates (LAS), which are used to formulate consumer products. Consumer exposure to LAB may occur due to residual amounts of LAB (typical ranges estimated to be from 0.1 - 1%) that remain in LAS (Takada and Ishiwatari, 1987; AIS, 1995). A “worst case” consumer dose estimate, of approximately 6.1×10^{-3} mg LAB/kg/day for consumer exposure to LAB was derived using the USES Version 1.0 dermal exposure model and oral uptake model described in the ECETOC Technical Report #58. The combined oral and dermal dose was estimated (AIS, 1995; European Union, 1997). Further details of this estimate are given in Appendix 2.

3. EFFECTS ON HUMAN HEALTH

3.1 Toxicokinetics and Metabolism

The distribution, metabolism and excretion of 1 mg/kg body weight of 2-(^{14}C)-phenyldodecane (PD) was studied in male and female rats after intravenous (IV), oral and dermal administration (Hazelton Europe, 1994a, 1994b, 1994c). The results of these studies are summarized below.

Intravenously administered PD was rapidly eliminated, principally in the urine. Metabolism of PD was rapid and extensive. Residual amounts of PD or its metabolites were observed in tissues with high lipid content.

Orally administered PD was rapidly and extensively absorbed. PD was excreted principally via urine, but also to some extent in the bile. Residual amounts of PD or its metabolites were observed in tissues with high lipid content.

Dermally administered PD was absorbed slowly and eliminated principally via urine. Only tissues having a high lipid content displayed some accumulation of the compound and/or its metabolites. Metabolism of PD was extensive with little or no unchanged test material present in the urine.

3.2 Acute Toxicity

Animal Data

LAB is practically non-toxic after a single dose by the oral (LD_{50} >5 g/kg) and dermal (LD_{50}, typically >2 g/kg) routes. Median lethal doses are presented in Table 1. The LC_{50} value in rats after a four-hour inhalation exposure to Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) was greater than 1.82 mg/L (Monsanto Report ML-80-71A).

Table 1. Acute toxicity of linear alkylbenzenes in experimental animals

Route	Species	Value	Type	Reference
Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})				
oral	rat	17,000 mg/kg	LD_{50}	Monsanto Report BT 65-2
inhal.	rat	>1.82 mg/L	LC_{50}	Monsanto Report ML-80-71A
dermal	rabbit	>10,200 mg/kg	LD_{50}	Monsanto Report BT 65-2
Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})				
oral	rat	28,200 mg/kg	LD_{50}	Monsanto Report BT 65-3
dermal	rabbit	>10,200 mg/kg	LD_{50}	Monsanto Report BT 65-3

Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})				
oral	rat	20,800 mg/kg	LD_{50}	Monsanto Report BT 65-4
dermal	rabbit	>10,200 mg/kg	LD_{50}	Monsanto Report BT 65-4
Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})				
oral	rat	>34,080 mg/kg	LD_{50}	CSL No. 6589-67
inhal.	rat	71 mg/L (nom)	LC_{50}	CSL No. 6589-67
dermal	rabbit	~2,000 mg/kg	LD_{50}	CSL No. 6589-67
dermal	rabbit	>5,000 mg/kg	LD_{50}	RT LAB. No. 871188
Nalkylene 600 (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})				
oral	rat	>35,800 mg/kg	LD_{50}	S.A. 202093
Nalkylene 600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})				
oral	rat	>5,000 mg/kg	LD_{50}	RT LAB No. 925621
dermal	rabbit	>2,000 mg/kg	LD_{50}	RT LAB. No. 925621
Nalkylene 550L (<1% C_9, 14% C_{10}, 30% C_{11}, 29% C_{12}, 20% C_{13}, 7% C_{14}, <1% C_{15})				
oral	rat	>5,000 mg/kg	LD_{50}	RT LAB No. 925620
dermal	rabbit	>2,000 mg/kg	LD_{50}	RT LAB. No. 925620

3.3 Irritation

Animal data

Linear alkylbenzenes are slightly irritating to the rabbit eye and slightly to moderately irritating to rabbit skin after single applications. Draize scores for skin and eye irritation in rabbits are presented in Table 2.

Table 2. Skin and eye irritation from linear alkylbenzenes in experimental animals

Route	Species	Draize Score	Exp. time	Reference
Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})				
skin	rabbit	3.8/8.0	72 hr	Monsanto Report BT-65-2
eye	rabbit	20.8/110	1 hr	Monsanto Report BT-65-2
Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})				
skin	rabbit	3.6/8.0	24 hr	Monsanto Report BT-65-3
eye	rabbit	14.4/110	1 hr	Monsanto Report BT-65-3

Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})				
skin	rabbit	3.0	24 hr	Monsanto Report BT-65-4
eye	rabbit	11.8/110	1 hr	Monsanto Report BT-65-4
Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})				
skin	rabbit	3.6	48 hr	CSL No. 6589-67
skin	rabbit	4.6	24 hr	RT LAB. No. 871188
eye	rabbit	2.0	1 hr	CSL No. 6589-67
Nalkylene 600 (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})				
skin	rabbit	2.4	24 hr	S.A. 202093
eye	rabbit	5.3	3 hr	S.A. 202093
Nalkylene 600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})				
skin	rabbit	2.5	24 hr	RT LAB. No. 925621
eye	rabbit	0.7	24 hr	RT LAB. No. 925621
Nalkylene 550L (<1% C_9, 14% C_{10}, 30% C_{11}, 29% C_{12}, 20% C_{13}, 7% C_{14}, <1% C_{15})				
skin	rabbit	3.6	24 hr	RT LAB. No. 925620
eye	rabbit	0	-	RT LAB. No. 925620

Human data

A human repeat insult patch test found that undiluted Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) was a primary and cumulative irritant in 149 of 205 individuals tested (Monsanto Report SH-81-1).

3.4 Sensitization

Animal data: Sensitization tests have been conducted on guinea pigs (Hüls, 1983). In the induction phase, the test animals (20, test and control) received three pairs of simultaneous, intradermal injections of 0.1 ml Freunds complete adjuvant (FCA), and 1 ml of 20% or 40% test substance (benzene C_{10}-C_{13} alkyl derivatives in paraffin oil). One week later, 50% test solutions were applied (under occlusion) to the same areas for 48 hours. Topical challenge occurred about 14 days later with 20% test substance (under occlusion). A second topical occluded challenge occurred about one week later (5% and 10% test solutions for 24 hours). None of the test animals exhibited sensitization reactions.

Human data

A human repeat insult patch test found that Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) was not a sensitizer in any of the 205 individuals tested (Monsanto Report SH-81-1).

3.5 Repeated Dose Toxicity

The results of repeated dose toxicity studies are summarized in Table 3. Rodents exposed to vapor concentrations of Alkylate 215 (340 and 830 mg/m^3), Alkylate 225 (105 and 293 mg/m^3) or Alkylate 230 (32, 97, and 308 mg/m^3) for 28 days, exhibited eye and nose irritation, decreased body weight gains and organ weight changes (Monsanto Report ML-80-71; Monsanto Report BD-84-277; Monsanto Report BD-84-315). No adverse microscopic effects were seen in the test animals. No-effect levels in these studies ranged from 0.03-0.1 mg/L. Rats exposed to Alkylate 215 showed similar signs of irritation and body weight changes in a 90-day inhalation study which resulted in a no-effect level of 0.l0 mg/L (Monsanto Report ML-82-1).

Exposure of rats to dietary levels of 2500-7500 ppm Alkylate 215 (equivalent to dose levels of about 200 to 2500 mg/kg) for 28 days resulted in reductions in body weight gain and food consumption.

Table 3. Repeated dose toxicity of linear alkylbenzenes in experimental animals

Sp.	Route	Exp. protocol	Critical Effects	Reference
Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})				
rat	inhal.	0. 100, 340, 830 mg/m^3 6 hr/day; 5 days/wk; 4 wk	NOAEL = 100 mg/m^3. Irrit. of eyes and nose, decreas. body wt. and changes in organ wts. at higher exposures. No histopathological changes	Monsanto Rpt. ML-80-71
rat	inhal	0. 102, 298, 580 mg/m^3 6 hr/day; 5 days/wk; ≤14 wk	NOAEL = 102 mg/m^3. Irrit. of skin and mucous membranes; respir. problems; decreas. body wt. gains at higher exposures. Liver wt. and enzymes elevated in high-dose females. No histopathological changes	Monsanto Rpt. ML-82-1
rat	oral/in diet	0, 2500, 5000, 7500, 20,000 ppm, in diet for 4 wk	NOAEL= <2500 ppm. Reduced body wt gain and food consumption at all doses	Monsanto Rpt. ML-80-58

Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})				
rat	inhal.	0. 29, 105, 293 mg/m^3 6 hr/day; 5 days/wk; 4 wk	NOAEL = 29 mg/m^3. Red nasal discharge at higher conc.; decreas. body wt. of males and increas. liver wts in females at 293 mg/m^3. No adverse histopathological changes	Monsanto Rpt. BD-84-277
Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})				
rat	inhal.	0. 32, 97, 308 mg/m^3 6 hr/day; 5 days/wk; 4 wk	Nasal discharge and lacrimation at all conc.; decreas. body wt. of males at all conc.	Monsanto Rpt. BD-84-315

3.6 Genetic Toxicity

Linear alkylbenzenes did not exhibit mutagenic activity in the Ames bacterial assay or in the CHO/HGPRT mammalian cell forward gene mutation assay. LAB exhibited no clastogenic activity in a rat bone marrow cytogenetics assay. A summary of the results of these studies is presented in Table 4.

Table 4. Results of genetic toxicity tests with linear alkylbenzenes

Test	Test System	Result	Reference
Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})			
Ames	S. typh. (strains TA98; TA100, TA1535, TA1537)	Negative with and without metabolic activation	Robinson and Nair, 1992
HGPRT	CHO (in vitro)	Negative with and without metabolic activation	Robinson and Nair, 1992
Chromosome aberration	Rat bone marrow (in vivo)	Negative	Robinson and Nair, 1992
Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})			
Ames	S. typh. (strains TA98; TA100, TA1535, TA1537)	Negative with and without metabolic activation	Robinson and Nair, 1992
HGPRT	CHO (in vitro)	Negative with and without metabolic activation	Robinson and Nair, 1992
Chromosome aberration	Rat bone marrow (in vivo)	Negative	Robinson and Nair, 1992
Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})			
Ames	S. typh. (strains TA98; TA100, TA1535, TA1537)	Negative with and without metabolic activation	Robinson and Nair, 1992
HGPRT	CHO (in vitro)	Negative with and without metabolic activation	Robinson and Nair, 1992

Chromosome aberration	Rat bone marrow (in vivo)	Negative	Robinson and Nair, 1992

3.7 Carcinogenicity

One investigator has reported that a linear alkylbenzene (described as a C_{12}-C_{20} monosubstituted LAB composed primarily of C_9 and C_{10} substituted components) promoted the production of lymphomas in a chronic skin painting study of dimethylbenzanthracene pre-treated mice (Iverson, 1990). The basis of this conclusion is unclear, particularly since the investigator combined different histological types of lymphoma. Furthermore, the use of high dermal concentrations of LAB, which would cause severe chronic injury to the skin such as ulceration and chronic dermatitis, also complicates the interpretation of this study. Prolonged epidermal hyperplasia has been shown to promote skin tumors in mice (Argyris, 1985). The use of excessive concentrations of skin irritants in chronic dermal bioassays is questionable.

3.8 Reproduction / Developmental Toxicity

Depressed weight gains in parental animals and decreases in litter size, pup viability, pup survival, and pup weight gains were observed in a two-generation reproduction study in which rats were exposed orally to Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) at dose levels of 0, 5, 50 and 500 mg/kg/day (Robinson and Schroeder, 1992). The NOEL for reproductive effects in offspring was 5 mg/kg, and the NOEL for parental toxicity was 50 mg/kg.

No abnormalities were found in rats in two developmental studies conducted on Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) (Robinson and Schroeder, 1992) and Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15}) (Monsanto Report BD-84-315). The test substances were administered orally in corn oil at dose levels of 0, 125, 500, or 2000 mg/kg on days 6 through 15 of gestation. The only effect observed was a depression of maternal weight gain which was statistically significant at the mid and high dose levels, and not at the low dose level of 125 mg/kg. The NOEL for developmental toxicity was 125 mg/kg.

3.9 Initial Assessment for Human Health

Linear alkyl benzenes do not present any significant acute or subchronic health effects by various exposure routes. LAB is not teratogenic and does not produce selective reproductive toxicity. Several short-term assays have found LAB to be non-mutagenic and non-clastogenic. Thus, LAB is unlikely to be a tumor initiator. The human health significance of a reported tumor promoting effect for a LAB is unclear, particularly, in face of the uncertainties introduced by the design of the study. Manufacturers warn workers against dermal contact and provide protective clothing to limit exposure. Exposure of consumers via cleaning products is extremely low. Comparison of the 5 mg/kg NOEL from the reproduction study

(Robinson and Schroeder, 1992) with the consumer exposure estimate of 6.1 x 10^{-3} mg/kg/day (AIS, 1995; European Union, 1997) yields a substantial safety margin of approximately 820.

4. EFFECTS ON THE ENVIRONMENT

4.1 Aquatic Effects

Linear alkylbenzenes, at concentrations up to and exceeding their water solubility limits, had no acute effects on all the species tested (*Pimphales promelas, Salmo gairdneri, Lepomis macrochirus, Gammarus fasciatus, Paratanytarsus parthenogenetica*, *Chironomus tentans*, *Mysidopsis bahia*, *Selenastrum capricornutum, Scenedesmus subspicatus*) except *Daphnia magna* (Gledhill et al., 1991). The 48-hour EC_{50} values for *Daphnia magna* ranged from 9 to 80 µg/L over the molecular weight range of commercial LAB's sold in the U.S. (Gledhill et al., 1991).

Linear alkylbenzenes are also probably more potent on a chronic basis to *Daphnia magna* than they are to the other species. Based on the results of acute toxicity tests (Table 5), linear alkylbenzenes are more than l0 times as toxic to daphnids as they are to fish, and because they are readily metabolized and eliminated by fish (Werner and Kimerle, 1982; Burke et al., 1991), it is highly unlikely that fish would be more sensitive than daphnids in chronic tests. Results of chronic toxicity tests are shown in Table 6. The lowest reported MATC for *Daphnia magna* is 7.5 µg/L for a 21-day exposure to Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14}) (Gledhill et al., 1991). In a partial chronic study (14 day duration), investigators observed no adverse effects in a study on chronimids, a typical sediment dwelling species, exposed to Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14}) at concentrations up to 125 µg/L (Gledhill et al., 1991). In tests conducted on fish (*Brachydanio rerio)*, the reported NOEC values for 14 and 21 day exposures were above the water solubility limits of the test substance, European Commercial LAB (Enichem Augusta Ind., 2001).

Table 5. Summary of acute effects on aquatic organisms

Species	Exposure duration	Results	Reference
Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})			
Fish:			
Salmo gairdneri	24-96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Pimephales promelas	24-96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Lepomis macrochirus	24-96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Daphnids: *Daphnia magna*	48 hr	EC_{50} = 0.08 mg/L	Gledhill et al., 1991
Mysid crustacean: *Mysidopsis bahia*	96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Amphipod crustacean: *Gammarus fasciatus*		No toxicity up to water solubility	Gledhill et al., 1991
Insects: *Paratanytarsus parthenogenetica*	48 hr	LC_{50} > water sol.	Gledhill et al., 1991
Algae: *Selenastrum capricornutum*	96 hr	EC_{50} > water sol.	Gledhill et al., 1991
Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})			
Fish: *Pimephales promelas*	24-96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Daphnids : *Daphnia magna*	48 hr	EC_{50} = 0.009 mg/L	Gledhill et al., 1991
Insects: *Chironomus tentans*	96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})			
Fish: *Pimephales promelas*	24-96 hr	LC_{50} > water sol.	Gledhill et al., 1991
Daphnids: *Daphnia magna*	48 hr	EC_{50} = 0.01 mg/L	Gledhill et al., 1991
European Commercial LAB (C_{10}-C_{13})			
Daphnids: *Daphnia magna*	48 hr 48 hrr	NOEC > water sol. NOEC > 40 µg/L.	Enichem Augusta Ind., 2001 Enichem Augusta Ind., 2001
Algae: *Scenedesmus subspicatus*	72 hr	NOEC ≥ 50 µg/L	Enichem Augusta Ind., 2001

Table 6. Summary of chronic effects on aquatic organisms

Species	Exposure duration	Results	Reference
Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})			
Daphnids: *Daphnia magna*	21 day	MATC= 7.5 µg/L	Gledhill et al., 1991
Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})			
Insects: *Chironomus tentans*	14 day	MATC = 125 µg/L	Gledhill et al., 1991
Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})			
Daphnids : *Daphnia magna*	21 days	MATC = 13 µg/L	Gledhill et al., 1991
European Commercial LAB (C_{10}-C_{13})			
Fish: *Brachydanio rerio*	14 days	NOEC > water sol.	Enichem Augusta Ind., 2001
	21 days	NOEC > 57.8 µg/L	Enichem Augusta Ind., 2001

The aquatic toxicity data in the literature (Gledhill et al., 1991) are based on commercial range LAB that consists of a mixture of homologs and isomers. If toxicity profiles for homologs of commercial LAB are estimated from water solubility and octanol/water partition coefficients information, remarkably good agreement with the observed values occurs (Nabholz, 1995).

4.2 Terrestrial Effects

No information is available.

4.3 Other Environmental Effects

No information is available

4.4 Initial Assessment for the Environment

4.4.1 Maximum Tolerated Concentration (MTC)

According to the provisional OECD guidelines, if chronic data are available for the most sensitive species tested in acute tests, then the Maximum Tolerated Concentration (MTC) is estimated by applying an

assessment factor of 10 to the chronic value. Applying these criteria to linear alkylbenzenes, the MTC = 0.0075 mg per liter/10 = 0.00075 mg/L = 0.75 ppb. If a very conservative assessment factor of 100 is used, the MTC = 0.075 ppb.

4.4.2 Aquatic Assessment

The highest concentration of LAB in the environment would be expected in the receiving waters of sewage treatment plants whose effluents go into small streams that provide the lowest dilutions. LAB concentrations in such waters were shown to range from non-detectable (< 0.1 µg/L) to 1 µg/L. If the MTC of 0.75 ppb is used, the ratios of MTC to the measured receiving water concentrations (Gledhill et al., 1991) exceeded one at all but two of the nine locations. These two locations use trickling filter wastewater treatment systems that are much less efficient in removing organics than the more widely used, activated sludge systems. The total BOD (biochemical oxygen demand) discharged at these plants would result in oxygen-depleted environments that are incompatible with aquatic life despite the presence of LAB. Even if the excessively conservative MTC of 0.075 ppb is used, the ratios of MTC to receiving water concentrations exceeded one in three of the nine locations and ranged from 2.7 to 5 in the activated sludge treatment locations (Gledhill et al., 1991).

4.4.3 Sedimentary Assessment

The highest concentrations of LAB are expected in the sediments of small streams that provide very low dilutions for the effluents of wastewater treatment plants. The highest measured concentration of LAB in sediments near such plants was 0.87 ppm (Gledhill et al., 1991). Dividing the sediment concentration by the measured soil partition coefficient normalized for soil organic carbon content (K_{oc} = 22,000), yields an estimated worst-case interstitial water concentration of 4.0×10^{-5} ppm or 4.0×10^{-2} ppb (0.87 ppm/22,000). For this worst-case situation, the ratio of the MTC to the interstitial water concentration 0.75 ppb/4×10^{-2} ppb = 19, or 1.9 if the excessively conservative 0.075 ppb MTC is used. These values suggest a low level of concern for organisms in sediments even in situations in which poorly treated wastewater goes into small streams that provide little dilution.

5. CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

Linear alkyl benzenes are very unlikely to present a risk to human health. The levels of both consumer and occupational exposure are expected to be very low based on their physical and chemical properties, use and handling patterns. LAB is not acutely toxic. Data from repeat exposure, reproductive and genotoxicity studies also suggest a low potential for toxic effects, therefore a low concern for both consumers and workers exposed to these materials.

LAB undergoes complete aerobic biodegradation and has little potential to bioconcentrate in fish due to its rapid metabolism. In addition, the low potential for release, results in estimated low levels of LAB in the environment that are of little concern for any adverse impact.
Based on these considerations, no additional data is needed to sufficiently characterize the health and environmental effects of LAB.

5.2 Recommendations

Linear alkylbenzenes are of low priority for further study

6. REFERENCES

AIS 1995. Consumer Exposure to LAB, Association Internationale de la Savonnerie (AIS), Brussels, 1995.

Argyris, T.S. 1985. Regeneration and the mechanism of epidermal tumor promotion. CRC Crit. Rev. Toxicol. 14(3): 211-258.

Bayona, J.M., J. Albaiges, A.M. Solanas and M. Grifol. 1986. Selective aerobic degradation of linear alkylbenzenes by pure microbial cultures. Chemosphere 15:595-598.

Burke, A.B., P. Millburn, K.R. Huckly and D.H. Hutson. 1991. Uptake and elimination from rainbow trout (Oncorhynchus mykiss) following exposure to [^{14}C-ring]-2-phenyldodecane. Environ. Toxicol. Chem. 10:1467-1477.

Cavalli, L., G. Cassani, J.Berna and A. Moreno. 1996a. Iso-branching of linear alkylbenzene sulphonate (LAS). Biodegradation study of two standard-models. Toxicol. Environ. Chem. 54: 167-186.

Cavalli, L., G. Cassani, M. Lazzarin, C. Maraschin, G. Nucci and L. Valtorta. 1996b. Iso-branching of linear alkylbenzene sulphonate (LAS). Tenside Surf. Det. 33:393-398.

Council of LAB/LAS Environmental Research, 1990. "Alkylbenzenes Summary of Safety Assessment", September, 1990.

Cozzarelli, I.M., R.P Eganhouse and M.J. Baedecker. 1990. Transformation of monoaromatic hydrocarbons to organic acids in anoxic groundwater environment. Environ Geol. Water. Sci. 16(2): 135-141.

CSL Report No. 6589-67

Dixie Services, Inc. 1991. Report No. 54142, Dec. 4, 1991

Eganhouse, R.P., D.L. Blumfield and I.R. Kaplan. 1983. Long-chain alkylbenzenes as molecular tracers of domestic wastes in the marine environment. Environ. Sci. Technol. 17:523-530.

Enichem Augusta Ind. (now Sasol Italy). 2001. HEDSET Data Sheet, CAS-No. 6774-74-7, EINECS-No. 267-051-0, Benzene C10-13 Alkyl derivs., last updated 22/03/01.

European Union. 1997. Risk Assessment Report, CAS No. 67774-74-7, Benzene, C10-13 Alkyl Derivs., European Union, June 1997.

Gledhill,W.E.,Saeger, V.W.and M.L. Trehy. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169 - 178

Grvbic-Galic, D. and T.M. Vogel. 1987. Transformation of toluene and benzene by mixed methanogenic cultures. Appl. Environ. Microbiol. 53(2): 254-260.

Hazelton Europe. 1994a. 2-(^{14}C)-Phenyldodecane: Phase 2, distribution (whole body autoradiography), metabolism and excretion following intravenous administration to the rat, Report No. 1016/2-1011.

Hazelton Europe. 1994b. 2-(^{14}C)-Phenyldodecane: Phase 3, distribution (whole body autoradiography), metabolism and excretion following oral administration to the rat, Report No. 1016/3-1011.

Hazelton Europe. 1994c. 2-(^{14}C)-Phenyldodecane: Phase 4, distribution (whole body autoradiography), metabolism and excretion following dermal application to the rat, Report No. 1016/4-1011.

Holt, M.S. 1992. Mineralisation of linear alkylbenzenes in soils and sludges. 3rd CESIO International Surfactants Congress and Exhibition - A World Market, Section E - Environment, June 1-5 1992, London, pp. 95-103.

Holt, M.S. and S.L. Berstein. 1992. Linear alkylbenzenes in sewage sludges and sludge amended soils. Water Res. 26(5): 613-624.

Hüls. 1983. "Prüfung auf hautsensibilisierende Wirkung am Meerschweinchen von Marlican," Hüls Report No. 1431983.

Iversen, O.H. 1990. Turmorigenesis and Carcinogenesis studies of a number of insulation oils and fluids and hairless and SENCAR mice with special reference to skin tumors and malignant lymphomas. APMIS Suppl. 13, Vol. 98, pp 3-60.

Kuhn, E.P., J. Zeyer, P.Eicher and R.P. Schwarzenbach. 1988. Anaerobic degradation of alkylated benzenes in denitrifying laboratory aquifer columns. Appl. Environ. Microbiol. 54(2): 490-496.

Major, D.W., C.I. Mayfield and J.F. Barker. 1988. Biotransformation of benzene by denitrification in aquifer sand. Groundwater 26(l): 8-14.

Nielsen, A.M., L.N. Britton, C.E. Beall, T.P. McCormick and G.L. Russell. 1997. Biodegradation of Coproducts of Commercial Linear alkylbenzene Sulfonate. Environ. Sci. Technol. 31(12): 3397-3404.

Monsanto Report ABC-27561

Monsanto Report BD-84-277

Monsanto Report BD-84-315

Monsanto Report BT-65-2

Monsanto Report BT-65-3

Monsanto Report BT-65-4

Monsanto Report HL-84-290

Monsanto Report ML-80-58

Monsanto Report ML-80-71

Monsanto Report ML-80-71A

Monsanto Report ML-82-1

Monsanto Report MO-810174. Acute Toxicity of Alkylate 215 to the Midge (*Paratanytarsus parthenogenetica*).

Monsanto Report SH-81-1

Monsanto Study ES-81-SS-41

Nabholz, J.V. 1995. Letter from Dr. J.V. Nabholz, U.S.Environmental Protection Agency, to Dr. A.M. Nielsen, Vista Chemical Company, 15 March 1995.

Radian Corp. and Versar, Inc. 1995. Preliminary Exposure Profile, Linear Alkylbenzenes, Final Report submitted to the U.S. Environmental Protection Agency by Radian Corporation and Versar, Inc., May 1, 1995, available on the Internet at www.epa.gov/opptintr/sids/lin_alk/usexposure.wpd.

Robinson, E.C. and R.S. Nair. 1992. The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery. Fund. Appl. Toxicol 18, 540-548. Based on Monsanto Report DA-79-367

Robinson, E.C. and R.E. Schroeder. 1992. Reproductive and developmental toxicity studies of a linear alkylbenzene mixture in rats. Fund. Appl. Toxicol. 18: 549-556.

RT LAB No. 871188

RT LAB No. 925620

RT LAB No. 925621

S.A. Report 202093

Schreiber, A.F. and U.K. Winkler. 1983. Transformation of tetralin by whole cells of Pseudomonas stutzeri AS39. Eur. J. Appl. Microbiol. Biotechnol. 18:6-10.

Sikkema, J and J.A.M.de Bont. 1991. Isolation and initial characterization of bacteria growing on tetralin. Biodegradation 2:15-23.

Takada, H. and R. Ishiwatari. 1987. Linear alkylbenzenes in urban riverine environments in Tokyo: distribution, source and behavior. Environ. Sci. Technol. 21: 875-883.

Takada, H. and R. Ishiwatari. 1990. Biodegradation experiments of linearalkybenzenes (LABs): isomeric composition of C_{12} LABs as an indicator of the degree of LAB degradation in the aquatic environment. Environ. Sci. Technol. 24(l): 86-91.

Takada, H., R. Ishiwatari and N. Ogura. 1992. Distribution of linear alkylbenzenes (LABs) and linear alkylbenzene sulfonates(LAS) in Tokyo bay sediments. Estuarine, Coastal and Shelf Sci. 35: 141-156.

USEPA. 1994. Guidelines for Completing the Initial Review Exposure Report, Final Draft, Environmental Exposure Branch, U.S. Environmental Protection Agency, March 1, 1994.

Valls, M., J.M. Bayona and J. Albaiges. 1989. Use of trialkylamines as an indicator of urban sewage in sludges, coastal waters and sediments. Nature 337:722-724.

Vista Analytical Report

Vista Chemical Company. 1991. Report 5412, December 4, 1991 (unpublished).

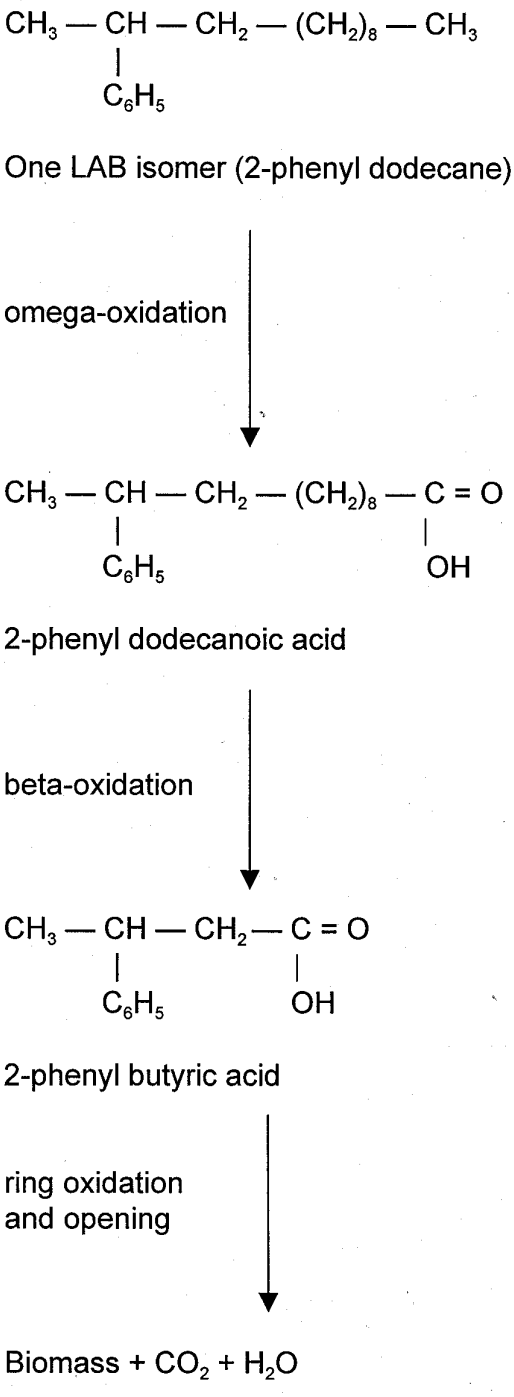
Werner, F. and R.A. Kimerle. 1982. Uptake and distribution of C_{12} alkylbenzene in bluegill (*Lepomis macrochirus*). Environ. Toxicol. Chem. 1:143-6.

Werner, A.F. and R.A. Kimerle. 1982. Uptake and distribution of C_{12} alkylbenzene in bluegill (Lepomis macrochirus). Environ. Toxicol. Chem. 1:143-146.

Wilson, B.H., G.B. Smith and J.F. Rees. 1986. Biotransformations of selected alkylbenzenes and halogenated aliphatic hydrocarbons in methanogenic aquifer material: a microcosm study. Environ. Sci. Technol. 20(10): 997-1002.

Zeyer, J., E.P. Kuhn and R.P. Schwarzenbach. 1986. Rapid microbial mineralization of toluene and 1,3-dimethylbenzene in the absence of molecular oxygen. Appl. Environ. Microbiol. 52(4): 944-947.

Appendix 1
Biodegradation Pathway of LAB



Appendix 2

Consumer Exposure to LAB

Hand dishwashing, hand washing of clothing and the use of dishes or other cooking utensils after dishwashing were considered in this assessment because these are the activities that provide the greatest chance of consumer exposure to LAB. The models used were those suggested in the EU Technical Guidance Document. These models provide "worst-case" estimates, assuming 100% oral or dermal uptake and using the highest values within a range of possible values for each exposure factor. Furthermore, typical events such as rinsing and wiping which would reduce the level of exposure were not taken into account.

I. Dermal exposure assessment during hand dishwashing and hand washing of laundry (USES Version 1.0 model)

The concentration of LAB in the solutions that consumers are exposed to is calculated as follows:

Hand dishwashing, average solution concentration = amount of product used (15 g) x fraction of LAB in product (0.0015) x end volume of dishwashing solution (5000 cm^{-3}) = 4.5 x 10^{-3} mg LAB/cm^3.

Handwashing of Laundry, average solution concentration = concentration of LAS in wash solution (1.2 g/L) x fraction of LAB in LAS (0.01) = 1.2 x 10^{-2} mg LAB/cm^3.

Dermal uptake = Average solution concentration x thickness of film layer x area of exposed skin x dermal uptake fraction x number of events per period/body weight.

1) For hand dishwashing, dermal uptake = 4.5 x 10^{-3} mg LAB x 0.01 cm x 1980 cm^2 x 1 x 2/70 kg x cm^3 = 2.5 x 10^{-3} mg LAB/kg body weight/day.

2) For hand washing of laundry, dermal uptake = 1.2 x 10^{-2} mg LAB x 0.01 cm x 1980 cm^2 x l x 1/70 kg x cm^3= 3.4 x 10^{-3} mg LAB/kg body weight/day.

Total dermal exposure (1 + 2) = 5.9 x 10^{-3} mg/kg body weight/day.

Appendix 2 (continued)

Consumer Exposure to LAB

II. Oral exposure due to deposits on dishes, cooking utensils, etc., after dishwashing:

A model in the ECETOC Technical Report #58 was used to estimate oral exposure to LAB. The assumes that all the residue remaining on the dish is reabsorbed during re-use of the dish and that the substance is then completely bioavailable once ingested by the consumer. Consequently, the calculation is very conservative.

1) Concentration of LAB in wash solution = maximum fraction of LAB in LAS (0.01) x fraction of LAS in a dishwashing product (0.15) x maximum product use concentration for dishwash (0.3% = 0.003 g/cm^3) = **4.5×10^{-3} mg/cm^3.**

2) Amount deposited per unit area = concentration of LAB in wash solution (4.5×10^{-3} mg/cm^3) x wash solution volume remaining on plate (0.25 cm^3) / the area of one side of a plate (450 cm^2) = 2.5×10^{-6} mg LAB/cm^2.

Amount of substance ingested = amt. deposited per unit area (2.5×10^{-6} mg LAB/cm^2) x fraction of deposited substance ingested (1) x utensils used per day (12) x area of dishes in contact with substance (450 cm^2) x body $weight^{-1}$ (70 kg) = **1.9×10^{-4} mg LAB/kg body weight/day.**

III. Total Consumer exposure estimate = Total dermal exposure estimate (5.9×10^{-3} mg/kg body weight/day) + oral exposure estimate (1.9×10^{-4} mg LAB/kg body weight/day) =
6.1×10^{-3} mg/kg body weight/day.

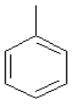
Appendix 3

Linear Alkylbenzenes Test Plan

Category Rationale/Justification:

The linear alkylbenzene (LAB) category is comprised of nine different commercial formulations found in Table 1. Each formulation is a mixture containing various proportions of individual LABs with the following formulae:

$$CH_3 - (CH_2)_x - CH - (CH_2)_y - CH_3$$



Where x + y = 7-13 and x = 0-7, giving a linear carbon range of C_{10} to C_{16}.

This category uses the "family of mixtures" approach and may further be subdivided into three subcategories based on the percentage of alkyl substituents with a low (C_{10}-C_{11}), mid (C_{11}-C_{13}), and high (C_{13}-C_{14}) proportion of carbon chain lengths.

Table 1
Assignment of LAB SubCategories[1]

LAB Formulation	Carbon Chain Length for Substituted Alkyl Group (Numbers represent percent of total)				
	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}[(2)]
Nalkylene 500	21	39	31	7	<1
Nalkylene 500L	20	44	31	5	<1
Alkylate 215	16	43	40	1	<1
Nalkylene 550L	14	30	29	20	7
Alkylate 225	7	25	48	19	1
Nalkylene 575L	9	17	20	30	15
Nalkylene 600	<1	1	23	50	25
Nalkylene 600L	<1	1	23	50	25
Alkylate 230	1	2	16	50	30

1 The shaded regions create three subcategories by presenting two ends of the spectrum in terms of a higher proportion (>50%) of shorter carbon chains (upper left) and a higher proportion (>50%) of longer carbon chains (lower right). Bolded formulations had available data in all SIDS categories.
2 The proportion of C_{15} and C_{16} is < 1% in all formulations except for an incidence of 1% C_{15} in Alkylate 230.

Matrix of SIDS endpoints indicating available/adequate data.

Study details for each required SIDS endpoint may be found in the dossier. The matrix provided in Table 2 is an analysis of the key available data (not all data) on the linear alkyl benzenes. Note that three LAB formulations (Alkylate 215, Alkylate 225, and Alkylate 230) had data available in each of the major SIDS classes (environmental fate, ecotoxicity, and health effects), and they each represent one of the three subcategories presented in Table 1. Table 3 indicates actual data to support the category rationale.

Table 2
STEP 4: Matrix of Available and Adequate Data on LAB CategoryMembers[1]

LAB Formulation	Environ-mental Fate	Ecological Effects			Human Health Effects			
		Fish Acute	Daphnid Acute	Daphnid Chronic	Acute[4]	Repeated Dose[5]	Mutagen-icity[6]	Develop-mental[7]
Nalkylene 500	-				√	-		
Nalkylene 500L					-			
Alkylate 215	√	√	√	√	√	-	√	√
Nalkylene 550L	-				√	-		
Alkylate 225	√	√	√	-	√	√	√	-
Nalkylene 575L	-				-			
Nalkylene 600	-				√	-		
Nalkylene 600L					√			
Alkylate 230	√	√	√	√	√	√	√	√

[1] "√" denotes data are available and adequate. "-" denotes data are either not available, or are available and are judged inadequate. Shaded areas mark the three subcategories identified in Table B-1.

Table 3
Evaluation of Matrix Data Patterns for LAB Category

LAB Formulation	Environ-mental Fate	Ecological Effects			Human Health Effects			
		Fish Acute	Daphnid Acute	Daphnid Chronic	Acute[4]	Repeated Dose[5]	Mutagenicity[6]	Develop-mental[7]
Nalkylene 500	Not tested	Not tested			>34 g/kg	Not tested		
Nalkylene 500L					Not tested			
Alkylate 215	**56%[1]**	**> Water solubility**	**80 ppb[2]**	**7.5 to 15 ppb[3]**	**17 g/kg**	**100 mg/m³**	**Negative**	**125 mg/kg**
Nalkylene 550L	Not tested	Not tested			>5 g/kg	Not tested		
Alkylate 225	**61%[1]**	**> Water solubility**	**9 ppb[2]**	**Not tested**	**28 g/kg**	**29 mg/m³**	**Negative**	**Not tested**
Nalkylene 575L	Not tested	Not tested			Not tested			
Nalkylene 600	Not tested	Not tested			>35 g/kg	Not tested		
Nalkylene 600L					>5 g/kg			
Alkylate 230	**56%[1]**	**> Water solubility**	**10 ppb[2]**	**13 to 23 ppb[3]**	**21 g/kg**	**<32 mg/m³**	**Negative**	**125 mg/kg**

[1] Percent of parent material evolved as carbon dioxide after 35 days in an aerobic biodegradation test.
[2] 48-hour LC_{50}s.
[3] 21-Day No Observed Effect Concentration (NOEC).
[4] Oral LD_{50}s in rodents.
[5] Four week inhalation studies in rats, values represent NOECs for the following effects: irritation of the eyes and nose and decreased body weight.
[6] Negative in vitro (bacteria - Ames; mammalian - Chinese hamster ovary cells) and in vivo (chromosomal aberration study in rats) tests.
[7] Developmental toxicity study (oral, rats, doses of 0, 125, 500, and 2000 mg/kg/d). Numbers in column represent no observed adverse effect level (NOAEL) for both maternal (weight gain) and developmental (ossification variations) endpoints.

Evaluation of data matrix patterns.

Adequate data are available for most endpoints for the three LAB formulations mentioned in Table 1. Table 3 presents the data values to validate the acceptability of the category rationale for each endpoint.

Table 3 indicates a consistent pattern of no discernible difference in aerobic degradation among the three LAB formulations tested (range of 56% - 61% of parent material evolved as carbon dioxide after a 35 day incubation period). Similarly, the acute fish toxicity, chronic daphnid toxicity, acute mammalian toxicity, reproductive/developmental toxicity, and mutagenicity data do not show differences across the tested formulations. However, the acute daphnid toxicity results, as well as the repeated dose toxicity tests in mammals suggest a pattern of increasing toxicity with an increase in the proportion of higher length carbon chains in the substituted alkyl group that appears to hold for each of these SIDS endpoints.

5. Conclusions/Recommendations

Based on the data evaluation, it was determined that the available data adequately represents the three separate formulations within the category boundaries. Existing data are sufficient for a screening level hazard assessment. As a result, we believe that no further testing is necessary under the SIDS programme.

STUDY CAS NO. 123-01-3 and 6742-54-7; (isomers: 68648-87-3, 139813-58-7, 68442-69-3, 129813-59-8, 151911-57-8 and 129813-60-1		INFO AVAIL	GLP	OECD STUDY	OTHER STUDY	ESTIM. METHODS	ACCEPT-ABLE	SIDS TESTING REQD
		Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
PHYSICAL/CHEMICAL								
2.1	Melting Point	Y	N	N	Y	N	Y	N
2.2	Boiling Point	Y	N	N	Y	N	Y	N
2.4	Vapor Pressure	Y	Y	N	Y	N	Y	N
2.5	Partition Coefficient	Y	N	N	N	Y	Y	N
2.6	Water solubility	Y	Y	N	Y	N	Y	N
OTHER STUDIES RECEIVED		Y	N	N	Y	N	Y	N
ENVIRONMENTAL FATE/ BIODEGRADATION								
3.1.1	Photodegradability	Y	N	N	Y	N	Y	N
3.1.2	Stability in Water	Y	N	N	Y	N	Y	N
3.2	Monitoring Data	Y	Y	N	Y	N	Y	N
3.3	Envir. Fate/Distribution	Y	N	N	N	Y	Y	N
3.5	Biodegradation	Y	N	N	Y	N	Y	N
3.7	Bioaccumulation	Y	Y	N	Y	Y	Y	N
OTHER STUDIES RECEIVED		Y	Y	N	Y	N	Y	N
ECOTOXICOLOGY								
4.1	Acute Toxicity - Fish	Y	Y	N	Y	N	Y	N
4.2	" - Daphnia	Y	N	N	Y	N	Y	N
4.3	" - Algae	Y	Y	N	Y	N	Y	N
4.4	Bacterial	N	--	--	--	--	--	N
4.5	Chronic aquatic organisms	Y	Y	N	Y	N	Y	N
4.6.1	Soil dwelling Organisms	N	--	--	--	--	--	N
4.6.2	Terrestrial Plants	N	--	--	--	--	--	N
4.6.3	Non-mammalian species Avian	N	--	--	--	--	--	N
OTHER STUDIES RECEIVED								
TOXICOLOGY								
5.1.1	Acute Oral	Y	N	N	Y	N	Y	N
5.1.2	Acute Inhalation	Y	N	N	Y	N	Y	N
5.1.3	Acute Dermal	Y	N	N	Y	N	Y	N
5.4	Repeated Dose	Y	Y	N	Y	N	Y	N
5.5	Genetic Toxicity	Y	Y	N	Y	N	Y	N
	" Gene Mutation	Y	Y	N	Y	N	Y	N
	" Chromosomal Aberrations	Y	Y	N	Y	N	Y	N
5.6	Genetic Toxicity In Vivo	Y	Y	N	Y	N	Y	N

5.7	Carcinogenicity	Y	N	N	Y	N	Y	N
5.8	Reproductive Toxicity	Y	Y	N	Y	N	Y	N
5.9	Developmental toxicity	Y	Y	N	Y	N	Y	N
5.10	Toxicokinetics	N	--	--	--	--	--	N
5.11	Human Experience	N	--	--	--	--	--	N

SIDS DOSSIER

Existing Chemical : Id._____

CAS No. : 123-01-3; 6742-54-7 (isomers 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 129813-60-1

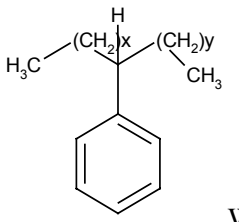
Chemical Name : undecylbenzene and dodecylbenzene; and Benzene, C_{10}-C_{16} alkyl derivative isomers

Molecular Formula : $C_6H_5C_nH_{2n+1}$ where n= 10-16.

Note : The information provided in this form refers to various mixtures of linear alkylbenzenes which are identified by the following CAS registry numbers: 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 129813-60-1
This information is submitted to fulfill the data submission requirements for the two materials designated by the CAS registry numbers, 6742-54-7 and 123-01-3. The attached Table I of the Appendix details the product composition of the various mixtures which represent the information presented in this submission.

1.01 SUBSTANCE INFORMATION

CAS Number : 123-01-3; 6742-54-7 (isomers 68648-87-3, 129813-58-7, 68442-69-3, 129813-59-8, 151911-57-8,129813-60-1
Name : Benzene, C_{10}-C_{16} alkyl derivative
Molecular Formula : $C_6H_5C_nH_{2n+1}$ where n= 10-16.
Structural Formula :



Where x + y = 7- 13 and x = 0-6

1.02 OECD INFORMATION

Sponsor Country : United States
Lead Organization : Environmental Protection Agency
Contact : Oscar Hernandez, Director RAD (7403M)
U.S. Environmental Protection Agency
1200 Pennsylvania Ave, Washington, DC 20460
Tel : 202 564-7641
Fax : 202 564-7430
E-mail hernandez.oscar@epa.gov
Name of Responder : Scott W. Waite
Research Chemist
Huntsman Corporation (successor to Monsanto Company LAB business)

David Penney
Senior Toxicologist
Sasol North America Inc (formerly Vista Chemical Company)

1.1 GENERAL SUBSTANCE INFORMATION

Substance Type : organic
Physical state : liquid
Purity : ≈87-99%
Source :

1.1.0 DETAILS ON TEMPLATE

1.1.1 SPECTRA

1.2 SYNONYMS

Linear alkylbenzene
LAB
Alkylate
Alkylate 215
Alkylate 225
Alkylate 229
Alkylate 230
Detergent alkylate

Nalkylene 550L
Nalkylene 600L
Nalkylene 500
Nalkylene 500L
Nalkylene 600
Nalkylene 575L
Nalkylene 580L

1.3 IMPURITIES

Dialkyltetralin
Isoalkylbenzene

1.4 ADDITIVES

Not applicable

1.5 QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.7 USE PATTERN

Remarks : By far, the major category of use for linear alkylbenzene is as an intermediate for the production of detergent surfactants. Estimates of greater than 98% of all LAB produced is consumed in the production of linear alkylbenzene sulfonate, a detergent surfactant. As such, use of linear alkylbenzene would be categorized as essentially all industrial use in closed systems.

1.7.1 TECHNOLOGY PRODUCTION/USE

1.8 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.9 SOURCE OF EXPOSURE

Remarks : The potential for exposure to linear alkylbenzenes in the real world is very limited, especially for consumers because only small amounts of LAB are present in final consumer products. Workers manufacturing linear alkylbenzene or other products containing linear alkylbenzenes have very low exposure. Low vapor pressure helps to diminish inhalation exposure and proper use of protective clothing for industrial workers limits potential for any skin or eye irritation. Even if small quantities are swallowed accidentally, or placed on the skin for a short period of time, it is very unlikely that linear alkylbenzenes would produce serious injury or harmful effect. Relatively high doses are required to induce acute, or immediate effects in laboratory tests, although the substance can irritate the eyes and skin.

Reference : Council of LAB/LAS Environmental Research, "Alkylbenzenes Summary of Safety Assessment", September, 1990. (1)

1.10.1 RECOMMENDATIONS/PRECAUTIONARY MEASURES

1.10.2 EMERGENCY MEASURES

1.11 PACKAGING

1.12 POSSIB. OF RENDERING SUBST HARMLESS

1.13 STATEMENTS CONCERNING WASTE

Remarks : Due to its nearly exclusive use as an industrial intermediate, disposal practices are limited to wastes or spills from industrial processing which are minor in nature. These wastes or spills are generally collected and incinerated using approved Incinerator operators.

1.14.1 WATER POLLUTION

1.14.2 MAJOR ACCIDENT HAZARDS

1.14.3 AIR POLLUTION

1.15 ADDITIONAL REMARKS

1.16 LAST LITERATURE SEARCH

1.17 REVIEWS

1.18 LISTING E.G. CHEMICAL INVENTORIES

2.1 MELTING POINT

Value : < -45.5°C
Sublimation :
Method :
Year :
GPL : no
Test Substance:
Remarks : Freezing Point not attained
Source :
Reference : Monsanto unpublished data
Flag : Cited in SIAR

Value : < -65°C
Sublimation :
Method : ASTM(D-97)
Year : 1991
GPL : no
Test Substance :
Remarks This is actually pour point temperature determination. The melting point is even lower
Source :
Reference: Dixie Services, Inc. Report No. 54142, Dec. 4, 1991(3)

Flag :

2.2 BOILING POINT

Value : 279°C (first drop); 283°C (10%); 287°C (50%); 291°C (90%); 295°C (endpoint)
Decomposition :
Method : ASTM D-86
Year :
GPL : no
Test Substance : Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks : At 101 kPa
Source :
Reference :
Monsanto unpublished data (21)
Flag : Cited in SIAR

Value : 277°C (first drop); 293°C (10%); 297°C (50%); 303°C (90%); 309°C (endpoint)
Decomposition :
Method : ASTM D-86
Year :
GPL : no
Test Substance : Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks : At 101 kPa
Source :
Reference: Monsanto unpublished data (21)
Flag : Cited in SIAR

Value : 279-292°C
Decomposition :
Method : ASTM D-86
Year :

GPL : no
Test Substance :N-600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15}), and N-500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks : At 101.325 kPa (1 atm)
Source :
Reference: Dixie Services, Inc. Report No. 54142, Dec. 4, 1991 (For N600L and N-500 only) (3)
Flag : Cited in SIAR

Value : 289-307°C
Decomposition :
Method : ASTM D-86
Year :
GPL : no
Test Substance : Alkylate 229 (<1%C_9, 1.1% C_{10}, 7.6% C_{11}, 36.4% C_{12}, 45.2% C_{13}, 9.6% C_{14}, <1%C_{15})
Remarks : At 101 kPa
Source :
Reference: Huntsman unpublished data
Flag : Updated April 2002

Value : 251-320°C
Decomposition :
Method : ASTM D-86
Year :
GPL : no
Test Substance : Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks : At 101 kPa
Source :
Reference: Huntsman unpublished data
Flag : Updated April 2002

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOR PRESSURE

Value : 6.5 x 10^{-5} kPa at 25°C (4.87 x 10^{-4} mmHg)
Decomposition :
Method : Measured
Year : 1991
GPL : yes
Test Substance : Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks : Vapor pressure reported as 4.9 x 10^{-4} mm Hg
Source :
Reference: Monsanto Report ABC-27561 (7)
Flag : Cited in SIAR
Value : <0.067-0.174 kPa at 21°C
Decomposition :
Method : Reid Method-ASTM(D323)
Year : 1991
GPL : no
Test Substance :
Remarks :
Source :
Reference: Dixie Services, Inc. Report No. 54142, Dec. 4, 1991 (3)

Flag :

2.5 PARTITION COEFFICIENT

log P_{ow} : 5.72-5.75 at 27°C
Method : calculated [log Kow = 5.2 - 0.68 log (solubility)]
Year : 1991
GPL :
Test Substance :
Remarks :
Source :
Reference: Gledhill, W.E., Saeger, V.W. and Trehy, M.L.1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169 – 178 (4)
Flag : Cited in SIAR

2.6.1 WATER SOLUBILITY

Value : 0.041 mg/l at 25°C
Method : Monsanto method
Year :
GPL : yes
Test Substance : Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks : Gas chromatographic determination: aqueous solubility was reported as the sum of the linear C9-13 alkylbenzene GC peak areas.
Source :
Reference: Monsanto Report ABC-27560 (6)
Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178 (4)
Flag : Cited in SIAR

2.6.2 SURFACE TENSION

2.7 FLASH POINT

Value : 135-137°C
Method : Cleveland Open Cup
Year :
GPL : no
Test Substance : Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks :
Source :
Reference: Monsanto unpublished data (21)
Flag :

Value : 138-157°C
Method : Cleveland Open Cup
Year :
GPL : no
Test Substance : Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks :
Source :
Reference: Monsanto unpublished data (21)
Flag :

Value : 143-156°C
Method : Pensky-Martens (D-73); closed cup
Year :
GPL : no
Test Substance :
Remarks :
Source :
Reference: Vista Analytical Report (27)
Flag :

2.8 AUTOFLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 ADDITIONAL REMARKS

Value : 7.1 x 10^2 torr-L/mole (9.34 x 10^{-4} atm-m^3/mol)
Method :
Year :
GPL :
Test Substance: for C_{12} linear alkylbenzene
Remarks : Henry's Law Constant
Source :
Reference: Monsanto Study ES-81-SS-41 (20)
Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178 (4)
Flag : Cited in SIAR

Value : 2.2 x 10^4
Method :
Year :
GPL :
Test Substance : for C_{12} linear alkylbenzene
Remarks : Soil/Water Partition Coefficient (K_{oc})
Source :
Reference: Monsanto Study ES-81-SS-41 (20)
Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178 (4)
Flag : Cited in SIAR

3.1.1 PHOTODEGRADATION

Type	:	
Light source	:	direct sunlight
Light spect.	:	
Rel. intensity	:	
Indirect photolysis	:	
Sensitizer	:	
Conc. of sens.	:	
Rate constant	:	
Degradation	:	<1% after 14 days
Deg. product	:	
Method	:	U.S. Environmental Protection Agency. 1979. Toxic Substances Control Act; Premanufacturing Testing of New Chemicals. Guidance for premanufacture testing. *Fed. Reg.* 44:16240-16292.
Year	:	1991
GPL	:	
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	Photochemical transformation studies of acetonitrile solutions of Alkylate 215 in direct sunlight indicated no significant direct photolysis or chemical transformation. Greater than 99% of the original material remained at the end of the 14-day test period in both the sunlight-exposed and dark control tubes.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

3.1.2 STABILITY IN WATER

Type	:	
Rate	:	0.076-0.170/day
Half-life	:	4-9 days
Concentration	:	100, 500 ppb
Deg. product	:	
Method	:	
Year	:	1991
GPL	:	
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	Loss attributed to microbial degradation
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

3.1.1 STABILITY IN SOIL

3.2 MONITORING DATA

Type of measurement : receiving waters, upstream and downstream from sewage treatment plants
Medium : water
Location : United States
Method :
Concentration : undetectable (<0.1 µg/l) to 0.5 µg/l (upstream), undetectable to 1.0 µg/l (downstream)
Substance :
Year : 1987-89 (collection date)
Remarks : 10 typical sewage plants throughout the United States were monitored
Source :
Reference : Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag : Cited in SIAR

Type of measurement : receiving waters, upstream and downstream from sewage treatment plants
Medium : sediment
Location : United States
Year 1987-89 (collection date)
Method :
Concentration : undetectable (<0.1 mg/kg) to 0.61 mg/kg (upstream), undetectable to 0.87 mg/kg (downstream)
Substance :
Remarks : 10 typical sewage plants throughout the United States were monitored. The plants were selected because their effluents receive low dilution in receiving waters (worst case in terms of final LAB concentrations in receiving water).
Source :
Reference : Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag : Cited in SIAR

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Type : Fugacity model using EPIWIN v 3.10 (level III)
Media : water, air, soil, sediment
Method : calculated
Environ. emissions : 1000 (kg/hr) for air, water, and soil (0 for sediment)
Parameters : mol. wt. = 246.44; Henry's Law Constant = 9.34 x 10^{-4} atm-m^3/mol; Log K_{ow} = 5.7 and Soil partition coefficient = 22,000; WS = 0.041 mg/L; BP = 279 C (median range of LABs); MP = –45C; t1/2 values (air) = 6.4 hrs, (water) = 96 hrs, (soil) = 96 hrs and (sediment) = 384 hrs
Year : 2002
Test Substance :
Result :

Distribution	(%)
Air	3.9
Water	38.4
Soil	54.4
Sediment	3.3

Remarks : It should be noted, that when using the EPIWIN model version 3.10 and entering the CAS number 123-01-3, the corresponding structure has the benzene ring on the terminal carbon which is inconsistent with the actual structure as defined in section 1 of the SIAR (the benzene ring is located on any carbon besides the terminal carbon.) As a result, the CAS number

input is not valid when using EPIWIN and the structure was input manually with the benzene ring being located on the third carbon.

Reference : U.S. EPA, model run using EPIWIN (SRC) version 3.10, May, 2002. (30)
Flag : Cited in SIAR.

3.4 MODE OF DEGRADATION IN ACTUAL USE

Method :
Year :
GPL :
Test Substance :
Remarks : Microbial metabolism is thought to be the primary degradation process for LAB in nature.
Source :
Reference : Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag : Cited in SIAR

3.5 BIODEGRADATION

Type : Aerobic
Inoculum :
Concentration : 18.2 mg/l
Contact time : 35-day test
Degradation : 56 ±8% (% CO_2 of theory evolved)
Result :
Deg. product :
Method : EPA 40 CFR 796.3100: Aerobic aquatic biodegradation
Year : 1991
GPL : no
Test Substance : Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks : tested in water
Source :
Reference : Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag :

Type : Aerobic
Inoculum :
Concentration : 18.3 mg/l
Contact time : 35-day test
Degradation : 61 ±8% (% CO_2 of theoretical evolved)
Result :
Deg. product :
Method : EPA 40 CFR 796.3100: Aerobic aquatic biodegradation
Year : 1991
GPL : no
Test Substance : Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks : tested in water
Source :
Reference : Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag :

Type : Aerobic
Inoculum :

Concentration	:	19.7 mg/l
Contact time	:	35-day test
Degradation	:	56 ±9% (% CO_2 of theory evolved)
Result	:	
Deg. product	:	
Method	:	EPA 40 CFR 796.3100: Aerobic aquatic biodegradation
Year	:	1991
GPL	:	no
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	tested in water
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	

Type	:	Activated sludge sewage treatment plant
Result:	:	Average percent removal >98%.
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

Type	:	Trickling filter sewage treatment plant
Result:	:	Average percent removal 69%.
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

3.7 BIOACCUMULATION

Species	:	Lepomis macrochirus
Exposure period	:	96 hr
Concentration	:	0.092 mg/L
Type of test	:	flow-through
BCF	:	35
Uptake	:	K1 = 12 L/mg/day
Elimination	:	K2 = 0.34/day
Country	:	
Method	:	ASTM. 1979. Proposed standard practice for conducting bioconcentration tests with fishes and saltwater bivalve molluscs. ASTM Committee E-35.21, Draft No. 9, April 13, 1979. 40 p.
Year	:	1982
GPL	:	yes
Test Substance	:	96.5% pure C_{12} Alkylbenzene
Remarks	:	Bioconcentration factor was measured as 35 but was calculated from the water solubility to be 6250-6600. The much smaller actual versus calculated value due apparently to LAB being metabolized and eliminated.
Source	:	
Reference	:	Werner, F. and R.A. Kimerle. 1982. Uptake and distribution of C_{12} alkylbenzene in bluegill (*Lepomis macrochirus*). Environ. Toxicol. Chem. 1:143-6. (28)
Flag	:	Cited in SIAR

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type	:	static
Species	:	Salmo gairdneri
Exposure period	:	24-96 hr
Unit	:	
Analytical monitoring	:	
LC_{50}	:	24hr, 48hr, 72hr, 96hr LC50 > water solubility
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	24, 48 hr values calculated using the probit method; 72 hr and 96 hr values calculated using the binomial method. All values are nominal concentrations.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

Type	:	static
Species	:	Pimephales promelas
Exposure period	:	24-96 hr
Unit	:	
Analytical monitoring	:	
LC_{50}	:	24hr, 48hr, 72hr, 96 hr LC50 > water solubility
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	All values calculated using the binomial method. All values are nominal concentrations.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

Type	:	static
Species	:	Pimephales promelas
Exposure period	:	24-96 hr
Unit	:	
Analytical monitoring	:	
LC_{50}	:	24hr, 48hr, 72hr, 96 hr LC50 > water solubility
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	All values calculated using the binomial method. All values are nominal concentrations.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static

Species	:	Pimephales promelas
Exposure period	:	24-96 hr
Unit	:	
Analytical monitoring	:	
LC_{50}	:	24hr, 48hr, 72hr, 96 hr LC50 > water solubility
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	All values calculated using the binomial method. All values are nominal concentrations.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Lepomis macrochirus
Exposure period	:	24-96 hr
Unit	:	
Analytical monitoring	:	
LC_{50}	:	24hr, 48hr, 72hr, 96 hr LC50 > water solubility
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	All values calculated using the moving average method. All values are nominal concentrations.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	semi-static
Species	:	Brachydanio rerio
Exposure period	:	14 days
Unit	:	
Analytical monitoring	:	yes
NOEC	:	> water solubility
Method	:	European Directive 84/449/EEC, C.1
Year	:	1999
GPL	:	yes
Test Substance	:	European Commercial LAB (C10-C13 LAB, average alkyl chain length 11.1-11.8)
Remarks	:	Results: No effects were observed for the concentrations tested. Both the LOEC and NOEC were higher than the solubility concentration. A decrease in the test substance concentration was observed within 24 hours (day 1 and day 14), but the daily renewal of test solutions guaranteed the exposure to the test substance. Test conditions: 1 g/L of LAB was added to reconstituted water; this was stirred for 24 hours and then transferred to a separatory funnel and allowed to stand 4 hours. The lower portion was slowly filtered (0.45 um HV Millipore) and used for testing and for dilutions (2:1 and 1:1). The test was performed with duplicate test vessels and a control in semi-static conditions with daily renewal of test and control solutions. Analytical determinations were performed by GC at t=0 and t=24 on day 1 and day 14.
Source	:	

Reference	:	HEDSET Data Sheet, CAS-No. 6774-74-7, EINECS-No. 267-051-0, Benzene C10-13 Alkyl derivs., Prepared by Enichem Augusta Ind. (now Sasol Italy), last updated 22/03/01
Flag	:	Updated April 2002
Type	:	flow through
Species	:	Brachydanio rerio
Exposure period	:	21 days
Unit	:	micrograms per liter
Analytical monitoring	:	yes
NOEC	:	> 57.8 ug/L
Method	:	OECD Guideline 203
Year	:	2000
GPL	:	yes
Test Substance	:	European Commercial LAB (C10-C13 LAB, average alkyl chain length 11.1-11.8), phenyl-C10 (C10-LAB), phenyl-C12 (C12-LAB), and phenyl-C18.
Remarks	:	Results: No effects were observed for C10-C13 LAB or the other test substances within 21 days at the concentrations tested, which were far above or close (pheny-C18) to the solubility limits. Test conditions: Acetone was used as a solvent (final concentration < 100 ug/L). Duplicate vessels for test solutions and solvent controls were used in a flow through test. Analytical determinations were performed daily by GC-MS. Mean concentrations (ug/L) were: C10-C13 LAB, 57.8; phenyl-C10 (C10-LAB), 78.7; phenyl-C12 (C12-LAB), 353.7; phenyl-C18, 7.8.
Source	:	
Reference	:	HEDSET Data Sheet, CAS-No. 6774-74-7, EINECS-No. 267-051-0, Benzene C10-13 Alkyl derivs., Prepared by Enichem Augusta Ind. (now Sasol Italy), last updated 22/03/01
Flag	:	Updated April 2002

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

Type	:	static
Species	:	Daphnia magna
Exposure period	:	48 hr
Unit	:	mg/L
Analytical monitoring	:	based on nominal concentration
EC_{50}	:	0.08 mg/L (48 hr);
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	A computer program was used to calculate the LC50 through three options. In order of preference: moving average angle analysis, probit analysis, and binomial probability. The method selected is determined by the characteristics of the database. The computer identifies which is the most preferred statistical method and performs the analysis.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Daphnia magna
Exposure period	:	48 hr
Unit	:	mg/L
Analytical monitoring	:	based on nominal concentration
EC_{50}	:	0.009 mg/L (48 hr);

Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	A computer program was used to calculate the LC50 through three options. In order of preference: moving average angle analysis, probit analysis, and binomial probability. The method selected is determined by the characteristics of the database. The computer identifies which is the most preferred statistical method and performs the analysis.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Daphnia magna
Exposure period	:	48 hr
Unit	:	mg/L
Analytical monitoring	:	based on nominal concentration
EC_{50}	:	0.01 mg/L (48 hr)
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	no
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	A computer program was used to calculate the LC50 through three options. In order of preference: moving average angle analysis, probit analysis, and binomial probability. The method selected is determined by the characteristics of the database. The computer identifies which is the most preferred statistical method and performs the analysis.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Mysidopsis bahia (Crustacea)
Exposure period	:	
Unit	:	
Analytical monitoring	:	
LC_{50}	:	96 hr LC50 > water solubility
MATC	:	
Method	:	ASTM E-35 on Pesticides. 1980. Standard Practice E729-80, Standard Practice for Conducting Acute Toxicity Tests with Fishes, Macroinvetebrates and Amphibians. 25p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Gammarus fasciatus (Crustacea)
Exposure period	:	

Unit	:	
Analytical monitoring	:	
LC_{50}	:	No toxicity up to water solubility
MATC	:	
Method	:	
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Paratanytarsus parthenogenetica (Insecta)
Exposure period	:	
Unit	:	
Analytical monitoring	:	
LC_{50}	:	48 hr LC50 > water solubility
MATC	:	
Method	:	
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Paratanytarsus parthenogenetica (Insecta)
Exposure period	:	
Unit	:	
Analytical monitoring	:	
LC_{50}	:	48 hr LC50 > water solubility
MATC	:	
Method	:	EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Monsanto Report # MO810174. Acute Toxicity of Alkylate 215 to the Midge (*Paratanytarsus parthenogenetica*). (18)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Chironomus tentans (Insecta)
Exposure period	:	
Unit	:	
Analytical monitoring	:	
LC_{50}	:	96 hr LC50 > water solubility
MATC	:	
Method	:	ASTM E-35 on Pesticides. 1980. Standard Practice E729-80, Standard Practice for Conducting Acute Toxicity Tests with Fishes, Macroinvetebrates and Amphibians. 25p.

Year	:	1991
GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Daphnia magna
Exposure period	:	48 hours
Unit	:	
Analytical monitoring	:	yes
NOEC	:	> water soluble concentration
Method	:	European Directive 84/449/EEC, C. 2
Year	:	1997
GPL	:	yes
Test Substance	:	European Commercial LAB (C10-C13 LAB, average alkyl chain length 11.1-11.8)
Remarks	:	Results: No effects of immobilization were found at the solubility concentration. Test conditions: 1 g/L of LAB was added to reconstituted water; this was stirred for 24 hours and then transferred to a separatory funnel and allowed to stand 4 hours. The lower portion was slowly filtered (0.45 um HV Millipore) and used for testing and for dilutions (2:1 and 1:1). The test was performed with duplicate vessels and a control. Analytical determinations were performed by GC at t=0 and t=48.
Source	:	
Reference	:	HEDSET Data Sheet, CAS-No. 6774-74-7, EINECS-No. 267-051-0, Benzene C10-13 Alkyl derivs., Prepared by Enichem Augusta Ind. (now Sasol Italy), last updated 22/03/01
Flag	:	Updated April 2002
Type	:	static
Species	:	Daphnia magna
Exposure period	:	48 hours
Unit	:	
Analytical monitoring	:	no
NOEC	:	> 0.04 mg/L (water-soluble concentration)
Method	:	European Directive 84/449/EEC, C. 2
Year	:	
GPL	:	yes
Test Substance	:	European commercial LAB (<1% <C_{10}, 9.4% C_{10}, 40.2% C_{11}, 32.7% C_{12}, 15.9% C_{13}, 0.9% C_{14})
Remarks	:	Results: No effects of immobilization were observed at the water-soluble concentration. Test conditions: 4 ml of the test substance was added to 3.2 L of deionized water and slowly stirred with a magnetic bar for 96 h. After this time, a 2-L aliquot was removed and the solubilized LAB extracted 3 times with n-hexane. The n-hexane extracts were combined and analyzed by GC-MS. The LAB concentrations tested were: 100, 75, 50, 25, and 12.5% of the saturated LAB solution (0.04 mg/L). Four replicates of each concentration were tested.
Source	:	
Reference	:	C. Verge et al., Acute toxicity of linear alkylbenzene (LAB) to Daphnia magna, Tenside Surf. Det. 36 (2), 127-129, 1999.
Flag	:	Updated April 2002
Type	:	semi-static

Species	:	Daphnia magna
Exposure period	:	144 hours
Units	:	micrograms per liter
Analytical monitoring	:	yes
NOEC	:	>100 ug/L (48 hours)
Method	:	OECD Guideline 202, part 1
Year	:	2000
GPL	:	yes
Test Substance	:	Phenyl-C4, phenyl-C8, phenyl-C10 (C10-LAB), phenyl-C12 (C12-LAB), phenyl-C14 (C14-LAB), phenyl-C16, phenyl-C18
Remarks	:	Results: EC50 values were calculated using Probit analysis. EC50 values at 48 hours for all the tested substances were above 100 ug/L. EC50 values at 96 hours were above 100 ug/L for the phenyl-C4 and C8 materials and above the estimated water solubility concentrations for the other test materials. EC50 values at 144 hours were above 100 ug/L for the phenyl-C4 and C8 materials, above the estimated water solubility concentrations for the phenyl-C14, C16 and C18 materials and below the estimated water solubility concentrations for the other test materials. Test conditions: Acetone was used as a solvent (final test concentrations <100 ug/L). Duplicate vessels for test solutions (12.5, 25, 50 and 100 ug/L), controls and solvent controls were used. The test and control media were replaced every two days.
Source	:	
Reference	:	HEDSET Data Sheet, CAS-No. 6774-74-7, EINECS-No. 267-051-0, Benzene C10-13 Alkyl derivs., Prepared by Enichem Augusta Ind. (now Sasol Italy), last updated 22/03/01
Flag	:	Updated April 2002

4.3 TOXICITY TO AQUATIC PLANTS, E.G. ALGAE

Species	:	Selenastrum capricornutum (algae)
Exposure period	:	
Unit	:	
Analytical monitoring	:	
EC_{50}	:	96 hr EC50 > water solubility
Method	:	Miller, W.E., Greene, J.C., and Shiroyama, T. 1978. The *Selenastrum capricornutum* Printz algal assay. EPA 600/9-78-018. Corvallis Environmental Reasearch Laboratories. U.S. Environmental Protection Agency, Corvallis, OR.
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR
Type	:	static
Species	:	Scenedesmus subspicatus
Endpoint	:	growth rate
Exposure period	:	72 hours
Units	:	micrograms per liter
Analytical monitoring	:	yes
NOEC	:	>/= 50 ug/L
LOEC	:	100 ug/L
EC_{50}	:	>100 ug/L
Method	:	OECD Guideline 201
Year	:	2000
GPL	:	yes

Test Substance	:	European Commercial LAB (C10-C13 LAB, average alkyl chain length 11.1-11.8), phenyl-C10 (C10-LAB), phenyl-C12 (C12-LAB), and phenyl-C14 (C14-LAB)
Remarks	:	Test conditions: Acetone was used as a solvent (final test concentrations 1mL/L). Triplicate vessels for test solutions (25, 50 and 100 ug/L) and 2-5 controls were used. Results: No effects were found for C10-C13 LAB at 50 ug/L, which is above the water solubility limit of 37.6 ug/L. EC50 values were above 100 ug/L for all the tested substances. Measured test concentrations (ug/L) were determined for phenyl-C12: Nominal Measured 25 23 50 25 100 48.
Source	:	
Reference	:	HEDSET Data Sheet, CAS-No. 6774-74-7, EINECS-No. 267-051-0, Benzene C10-13 Alkyl derivs., Prepared by Enichem Augusta Ind. (now Sasol Italy), last updated 22/03/01
Flag	:	Updated April 2002

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Type	:	flow-through
Species	:	Daphnia magna
Age	:	First instar (< 24 hr old)
Exposure period	:	21 days
Unit	:	µg/L
Analytical monitoring	:	
LC_{50}	:	12 µg/L
MATC	:	7.5 µg/L
Method	:	ASTM. 1979. Proposed Standard Practice for Conducting Renewal Life Cycle Toxicity Tests with Daphnids. Draft No. 5, September, 1979, ASTM Committee E-35.21. 4 p. EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.
Year	:	1991
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	reproduction and growth affected at concentration of 15 µg/L
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

Type	:	flow-through
Species	:	Daphnia magna
Age	:	first instar (<24 hr old)
Exposure period	:	21 days
Unit	:	µg/L
Analytical monitoring	:	All values are measured concentrations.
LC_{50}	:	
MATC	:	13 µg/L
Method	:	ASTM. 1979. Proposed Standard Practice for Conducting Renewal Life Cycle Toxicity Tests with Daphnids. Draft No. 5, September, 1979, ASTM Committee E-35.21. 4 p.

EPA. 1975. Methods for Acute Toxicity Tests with Fish, Macroinvertebrates and Amphibians. EPA-660/3-75-009. April 1975. 61p.

Year	:	
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	reproduction and growth affected at concentration of 23 µg/L
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

Type	:	flow-through
Species	:	Chironomus tentans (Insecta)
Exposure period	:	14-day
Unit	:	µg/l
Analytical monitoring	:	
LC_{50}	:	
MATC	:	No effects on survival or growth were observed up to and including the highest concentration (measured as 125 µg/l)
Method	:	Mosher, R.G., Kimerle, R.A., and Adams, W.J., MIC Environmental Assessment Method for Conducting 14-day Water Exposure Partial Life Cycle Toxicity Tests With the Midge *Chironomus tentans*, Monsanto Environmental Sciences Report No. ES-82-M-11, St. Louis, Missouri, 1982
Year	:	
GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	Test was a 14-day partial chronic study.
Source	:	
Reference	:	Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)
Flag	:	Cited in SIAR

4.6.1 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO OTHER NON-MAMM. TERRESTRIAL SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

Test Substance	:	LABs
System studied	:	Receiving water and sediments near 10 sewage treatment plants
Remarks	:	A safety assessment of LAB indicates that it has little potential to bioconcentrate in fish due to rapid metabolism. Safety margins were calculated for all of the monitored sites, and ranged from 8 to >75 for receiving waters and from 190 to >1650 for sediments. Values reported are considered worst case because data were collected in close proximity to sewage outfalls and from receiving waters providing low dilution for sewage effluents. In addition, true bioavailability (soluble LAB) was not established by separate determination of adsorbed and soluble material for effluent and receiving water samples. Aerobic biodegradation and sediment partitioning further downstream would continue to lessen the bioavailabiltiy of LAB.
Source	:	

Reference : Gledhill, W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169-178. (4)

Flag :

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	17,000 mg/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	Monsanto Report BT-65-2 (10)
Flag	:	Cited in SIAR

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	28,200 mg/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	Monsanto Report, BT-65-3 (11)
Flag	:	Cited in SIAR

Type	:	LD50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	20,800 mg/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	Monsanto Report, BT-65-4 (12)
Flag	:	Cited in SIAR

Type	:	LD50
Species	:	rat
Strain	:	Holtzman
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>34.08 g/kg
Method	:	
Year	:	
GPL	:	no

Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	CSL Report No. 6589-67 (2)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rat
Strain	:	Cox-SD
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>35.8 g/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 600 (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	S.A. 202093 (26)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rat
Strain	:	SD
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>5 g/kg
Method	:	
Year	:	
GPL	:	
Test Substance	:	Nalkylene 600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	RT LAB No. 925621 (25)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rat
Strain	:	SD
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>5 g/kg
Method	:	
Year	:	
GPL	:	
Test Substance	:	Nalkylene 550L (<1% C_9, 14% C_{10}, 30% C_{11}, 29% C_{12}, 20% C_{13}, 7% C_{14}, <1% C_{15})
Remarks	:	considered to be practically non-toxic
Source	:	
Reference	:	RT LAB No. 925620 (24)
Flag	:	Cited in SIAR

5.1.2 ACUTE INHALATION TOXICITY

Type	:	LC50
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>1.82 mg/l
Method	:	
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	administered as an aerosol
Source	:	
Reference	:	Monsanto Report ML-80-71A (16)
Flag	:	Cited in SIAR

Type	:	LC50
Species	:	rat
Strain	:	Holtzman
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	71 mg/l (nominal)
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	administered as an aerosol
Source	:	
Reference	:	CSL No. 6589-67 (2)
Flag	:	Cited in SIAR

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>10,200 mg/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	Monsanto Report, BT-65-2 (10)
Flag	:	Cited in SIAR

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>10,200 mg/kg
Method	:	
Year	:	

GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	Monsanto Report, BT-65-3 (11)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>10,200 mg/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1%C_{15})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	Monsanto Report, BT-65-4 (12)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand albino
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	approximately 2 g/kg
Method	:	
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	CSL No. 6589-67 (2)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand albino
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>5 g/kg
Method	:	
Year	:	
GPL	:	
Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	RT LAB. No. 871188 (23)
Flag	:	Cited in SIAR
Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand albino
Sex	:	
Number of animals	:	

Vehicle	:	undiluted
Value	:	>2 g/kg
Method	:	
Year	:	
GPL	:	
Test Substance	:	Nalkylene 600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1%C_{15})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	RT LAB. No. 925621 (25)
Flag	:	Cited in SIAR

Type	:	LD50
Species	:	rabbit
Strain	:	New Zealand albino
Sex	:	
Number of animals	:	
Vehicle	:	undiluted
Value	:	>2 g/kg
Method	:	
Year	:	
GPL	:	
Test Substance	:	Nalkylene 550L (<1% C_9, 14% C_{10}, 30% C_{11}, 29% C_{12}, 20% C_{13}, 7% C_{14}, <1%C_{15})
Remarks	:	considered practically nontoxic
Source	:	
Reference	:	RT LAB. No. 925620 (24)
Flag	:	Cited in SIAR

5.1.4 ACUTE TOXICITY OTHER ROUTES

5.2.1 SKIN IRRITATION

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum scores: 3.8/8.0 after 72 hrs
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	considered moderately irritating based on average score
Source	:	
Reference	:	Monsanto Report BT-65-2 (10)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	

Result	:	maximum scores: 3.6/8.0 after 24 hrs
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	considered moderately irritating based on average score
Source	:	
Reference	:	Monsanto Report BT-65-3 (11)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum score: 3.0 after 24 hrs
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1%C_{15})
Remarks	:	considered slightly irritating based on average score
Source	:	
Reference	:	Monsanto Report BT-65-4 (12)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum score: 3.6 at 48 hrs
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	CSL No. 6589-67 (2)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum score: 4.6 at 24 hrs
EC classification	:	

Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	
Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	RT. LAB No. 871188 (23)
Flag	:	Cited in SIAR
Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum score: 2.5 at 24 hrs
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	
Test Substance	:	Nalkylene 600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1%C_{15})
Remarks	:	
Source	:	
Reference	:	RT. LAB No.925621 (25)
Flag	:	Cited in SIAR
Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum score: 2.4 at 24 hrs
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 600 (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1%C_{15})
Remarks	:	
Source	:	
Reference	:	S.A. Report 202093 (26)
Flag	:	Cited in SIAR
Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
PDII	:	
Result	:	maximum score: 3.6 at 24 hrs
EC classification	:	

Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	
Test Substance	:	Nalkylene 550L (<1% C_9, 14% C_{10}, 30% C_{11}, 29% C_{12}, 20% C_{13}, 7% C_{14}, <1%C_{15})
Remarks	:	
Source	:	
Reference	:	RT LAB. No. 925620 (24)
Flag	:	Cited in SIAR

5.2.2 EYE IRRITATION

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum scores: 20.8/110 after 1 hr
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	considered slightly irritating based on average score
Source	:	
Reference	:	Monsanto Report BT-65-2 (10)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum scores: 14.4/110 after 1 hr
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	
GPL	:	no
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	considered slightly irritating based on average score
Source	:	
Reference	:	Monsanto Report BT-65-3 (11)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum scores: 11.8/110 after 1 hr
EC classification	:	
Method	:	Draize, J.H., Woodard, G., and Calvery, H.O.; J.Pharm. Exp. Ther, 82:4 (1944)
Year	:	

GPL	:	no
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	considered slightly irritating based on average score
Source	:	
Reference	:	Monsanto Report BT-65-4 (12)
Flag	:	Cited in SIAR
Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum score: 2.0 at 1 hr
EC classification	:	
Method	:	Draize
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 500 (1% C_9, 21% C_{10}, 39% C_{11}, 31% C_{12}, 7% C_{13}, <1% C_{14})
Remarks	:	considered non-irritating based on maximum average score
Source	:	
Reference	:	CSL. No. 6589-67 (2)
Flag	:	Cited in SIAR
Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum score: 0.7 at 24 hr
EC classification	:	
Method	:	Draize
Year	:	
GPL	:	
Test Substance	:	Nalkylene 600L (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})
Remarks	:	considered non-irritating based on maximum average score
Source	:	
Reference	:	RT. LAB. No. 925621 (25)
Flag	:	Cited in SIAR
Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum score: 5.3 at 3 hrs
EC classification	:	
Method	:	Draize
Year	:	
GPL	:	no
Test Substance	:	Nalkylene 600 (<1% C_9, <1% C_{10}, 1% C_{11}, 23% C_{12}, 50% C_{13}, 25% C_{14}, <1% C_{15})
Remarks	:	considered non-irritating based on maximum average score
Source	:	
Reference	:	S.A. 202093 (26)
Flag	:	Cited in SIAR

Species	:	rabbit
Strain	:	New Zealand
Concentration	:	undiluted
Exposure	:	
Exposure time	:	
Number of animals	:	
Result	:	maximum score: 0
EC classification	:	
Method	:	Draize
Year	:	
GPL	:	
Test Substance	:	Nalkylene 550L (<1% C_9, 14% C_{10}, 30% C_{11}, 29% C_{12}, 20% C_{13}, 7% C_{14}, <1% C_{15})
Remarks	:	considered non-irritating based on maximum average score
Source	:	
Reference	:	R.T. LAB. No. 925620 (24)
Flag	:	Cited in SIAR

5.3 SENSITIZATION

Type	:	Guinea Pig Maximization Test
Species	:	Guinea pig
Number of animals	:	20 (test and control)
Vehicle	:	paraffin oil
Result	:	0/20 test animals showed reactions indicative of sensitization
Method	:	OECD guideline 406, Skin Sensitization
Year	:	1992
GPL	:	no
Test Substance	:	Benzene C10-13 alkyl derivs. (CAS 67774-74-7)
Remarks	:	In the induction phase, test guinea pigs received three pairs of intradermal injections simultaneously. The paired injections were, (1) 0.1 ml Freunds complete adjuvant (FCA), (2) 0.1 ml 20% test substance in paraffin oil, (3) 0.1 ml 40% test substance in FCA. One week later, 2 X 4 cm filter papers soaked with 50% test substance in paraffin oil were applied to the same area of the shoulders and then held in place with occlusive dressing for 48 hours. This application was followed by topical challenge about 14 days later in which the left flanks of test animals were exposed to 2 X 4 cm filter papers soaked with 20% substance in paraffin oil, held in place with occlusive wrapping. A second topical challenge was also performed about one week later, in which the right flanks of the test animals were exposed to 2 X 2 cm filter paper strips soaked with 5% and 10% test substance in paraffin oil, held in place for 24 hours with an occlusive wrapping. Observations of skin reactions indicative of irritation or sensitization at each challenge were conducted at 24, 48 and 72 hours following the removal of occlusive wrappings.
Source	:	Cited in EU Risk Assessment Report, Revision June 1997, CAS No 67774-74-7, Benzene C10-13 Alkyl Derivs.
Reference	:	Hüls Report No. 143, “Prüfung auf hautsensibilisierende Wirkung am Meerschweinchen von Marlican,” 1983.
Flag	:	Updated April 2002

Species	:	human
Strain	:	
Dose	:	0.2 ml
Exposure	:	
Exposure time	:	
Number of individuals	:	205
Control group	:	none
Result	:	number of individuals with skin reaction at challenge: 0 of 205
Classification	:	

Method	:	volunteers were treated with a series of 24 hour applications (0.2 ml on the webril pad of an adhesive bandage) during the 3 week induction period and subsequent challenge phase.
Year	:	
GPL	:	no
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	The undiluted material was a primary irritant in 149/205 individuals. A diluted sample (50% Alkylate 215 in corn oil) was a primary irritant in 13 individuals. No individuals were considered to be sensitized to the diluted sample of test material.
Source	:	
Reference	:	Monsanto Report SH-81-1 (19)
Flag	:	Cited in SIAR

5.4 REPEATED DOSE TOXICITY

Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	4 weeks
Frequency of treatment	:	6 hr/day, 5 days/wk
Post obs. period	:	
Concentrations	:	0, 100, 340, and 830 mg/m^3
Control group	:	yes
Results	:	Irritation of the eyes and nose, decreased mean body weights and changes in organ weights or organ/body weight ratios were observed at the mid- and high-exposure concentrations. A loss of abdominal fat was noted at the highest concentration. No adverse histopathological changes were observed.
NOAEL	:	= 100 mg/m^3
Method	:	EPA/TSCA. Animals were observed and weighed during the study. Afterwards tissues were weighed and examined for histopathological changes
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Monsanto Report ML-80-71 (15)
Flag	:	Cited in SIAR

Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	up to 14 weeks
Frequency of treatment	:	6 hr/day, 5 days/wk
Post obs. period	:	
Concentrations	:	0, 102, 298, and 580 mg/m^3
Control group	:	yes
Results	:	Skin and mucous membrane irritation and respiratory problems were evident at the mid- and high-exposure concentrations. Body weight gains were also depressed at these levels. While liver weights and serum levels of hepatic enzymes were elevated in females in the highest-exposure group, there were no gross or histopathological changes.
NOAEL	:	= 102 mg/m^3

Method	:	EPA/TSCA. Animals were observed and weighed during the study. Afterwards tissues were weighed and examined for histopathological changes.
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Monsanto Report ML-82-1 (17)
Flag	:	Cited in SIAR
Species	:	rat
Sex	:	males and females
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	4 weeks
Frequency of treatment	:	6 hr/day, 5 days/wk
Post obs. period	:	
Concentrations	:	0, 29, 105, and 293 mg/m^3
Control group	:	yes
Results	:	Mid and high-exposure concentrations were associated with red nasal discharge. Body weights of males were depressed at the high-concentration, and liver weight of females were increased at this level. No adverse histopathological findings were noted.
NOAEL	:	= 29 mg/m^3
Method	:	EPA/TSCA. Animals were observed and weighed during the study. Afterwards tissues were weighed and examined for histopathological changes.
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	
Source	:	
Reference	:	Monsanto Report BD-84-277 (8)
Flag	:	Cited in SIAR
Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	inhalation
Exposure period	:	4 weeks
Frequency of treatment	:	6 hr/day, 5 days/wk
Post obs. period	:	
Concentrations	:	0, 32, 97, and 308 mg/m^3
Control group	:	yes
Results	:	Nasal discharge and lacrimation were increase in all exposure groups. Body weights of males were slightly depressed throughout the study.
NOAEL	:	
Method	:	EPA/TSCA. Rats were observed and weighed during the study. No histopathological evaluation was conducted
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	
Source	:	
Reference	:	Monsanto Report BD-84-315 (9)
Flag	:	Cited in SIAR
Species	:	rat

Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	oral
Exposure period	:	4 weeks
Frequency of treatment	:	daily, in diet
Post obs. period	:	
Concentrations	:	0, 2500, 5000, 7500, and 20000 ppm, in diet
Control group	:	yes
Results	:	Reductions in body weight and food consumption were noted at all exposure levels. No gross pathological changes were noted.
NOAEL	:	= <2500 ppm in diet, reduced weight gain observed at all doses
Method	:	EPA/TSCA. Rats were observed and weighed during the study. Histopathology was not carried out.
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Monsanto Report ML-80-58 (14)
Flag	:	Cited in SIAR

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	Bacterial test
System of testing	:	Salmonella typhimurium/TA-98,100,1535, and 1537
Concentration	:	
Cytotoxic conc.	:	with metabolic activation: 0.010 mg/plate without metabolic activation: 0.010 mg/plate
Conc. causing precip.	:	0.001 mg/plate
Metabolic activation	:	with and without
Result	:	negative with and without activation
Method	:	EPA/TSCA, plate incorporation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR

Type	:	Bacterial test
System of testing	:	Salmonella typhimurium/TA-98,100,1535, and 1537
Concentration	:	
Cytotoxic conc.	:	with metabolic activation: >10 mg/plate without metabolic activation: >10 mg/plate
Conc. causing precip.	:	3.0 mg/plate
Metabolic activation	:	with and without
Result	:	negative with and without activation
Method	:	EPA/TSCA, plate incorporation assay
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)

Flag	:	Cited in SIAR
Type	:	Bacterial test
System of testing	:	Salmonella typhimutium/TA-98,100,1535, and 1537
Concentration	:	
Cytotoxic conc.	:	with metabolic activation: >10 mg/plate without metabolic activation: >10 mg/plate
Conc. causing precip.	:	3.0 mg/plate
Metabolic activation	:	with and without
Result	:	negative with and without activation
Method	:	EPA/TSCA, plate incorporation assay
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR
Type	:	Non-bacterial test
System of testing	:	CHO/HGPRT point mutation
Concentration	:	
Cytotoxic conc.	:	with metabolic activation: 1.0 mg/ml without metabolic activation: 0.250 mg/ml
Conc. causing precip.	:	
Metabolic activation	:	with and without
Result	:	negative with and without activation
Method	:	EPA/TSCA, HGPRT point mutation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR
Type	:	Non-bacterial test
System of testing	:	CHO/HGPRT point mutation
Concentration	:	
Cytotoxic conc.	:	with metabolic activation: 0.5 mg/ml without metabolic activation: 0.5 mg/ml
Conc. causing precip.	:	
Metabolic activation	:	with and without
Result	:	negative with and without activation
Method	:	EPA/TSCA, HGPRT point mutation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR
Type	:	Non-bacterial test

System of testing	:	CHO/HGPRT point mutation
Concentration	:	
Cytotoxic conc.	:	with metabolic activation: 1.6 mg/ml without metabolic activation: 1.6 mg/ml
Conc. causing precip.	:	
Metabolic activation	:	with and without
Result	:	negative with and without activation
Method	:	EPA/TSCA, HGPRT point mutation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay (bone marrow chromosome abberation)
Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	Negative for genotoxicity Lowest dose producing toxicity: 6,000 mg/kg; Effect on Mitotic Index or P/N Ratio: no effect
Method	:	EPA/TSCA, bone marrow chromosome abberation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR

Type	:	Cytogenetic assay (bone marrow chromosome abberation)
Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	Negative for genotoxicity Lowest dose producing toxicity: 12,700 mg/kg; Effect on Mitotic Index or P/N Ratio: no effect
Method	:	EPA/TSCA, bone marrow chromosome abberation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 225 (<1% C_9, 7% C_{10}, 25% C_{11}, 48% C_{12}, 19% C_{13}, 1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)

Flag	:	Cited in SIAR
Type	:	Cytogenetic assay (bone marrow chromosome abberation)
Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	
Exposure period	:	
Doses	:	
Result	:	Negative for genotoxicity Lowest dose producing toxicity: 4,000 mg/kg; Effect on Mitotic Index or P/N Ratio: no effect
Method	:	EPA/TSCA, bone marrow chromosome abberation
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Nair, R.S.; The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery; Fund. Appl. Toxicol 18, 540-548 (1992). (22)
Flag	:	Cited in SIAR

5.7 CARCINOGENICITY

Species	:	mice
Sex	:	
Strain	:	Hairless hr/hr mice Oslo strain
Route of admin.	:	skin application
Exposure period	:	18 months
Doses	:	20 and 40% in µL100 acetone
Result	:	Enhanced mortality and skin effects (hyperplasia and pigment leakage) were observed. No complete carcinogenic activity was observed, however, a promoting effect on carcinogenesis but not tumorigenesis was reported.
Method	:	Two stage initiation/promotion protocol, initial single application 51.2 or 25.6 µL of 7, 12-dimethylbenzen(a)anthracene followed by skin application of test material at 20 and 40% in µL100 acetone for 18 months; complete carcinogenesis protocol, mice received twice weekly skin applications of 20, 40, or 80% test material in 100 µL acetone for 18 months.
Year	:	1990
GPL	:	no
Test Substance	:	described as a C12-C20 monosubstituted linear alkylbenzene composed primarily of C9 and C10 substituted components
Remarks	:	The interpretation of the study is confounded by the use of high concentrations of test material resulting in severe skin irritation. Epidermal hyperplasia has been shown to promote skin tumors in mice. (Argyria, T.S. Regeneration and the mechanism of epidermal tumor promotion. CRC Crit. Rev. Toxicol, 14(3), 211-258, 1985)
Source	:	
Reference	:	Iversen, O.H. Turmorigenesis and Carcinogenesis studies of a number of insulation oils and fluids and hairless and SENCAR mice with special reference to skin tumors and malignant lymphomas, APMIS Suppl. 13, Vol. 98, pp 3-60, 1990. (5)
Flag	:	Cited in SIAR

5.8 TOXICITY TO REPRODUCTION

Species	:	rat
Sex	:	
Strain	:	Sprague-Dawley
Route of admin.	:	oral
Exposure period	:	for 2 generations; during premating, mating, gestation, and lactation periods
Doses	:	0, 5, 50, and 500 mg/kg, administered in corn oil
Result	:	Reduced weight gain in parental animal and decrease in litter size, pup viability, pup survival, and pup weight gains were found at the high dose group. No consistent adverse effects of treatment were found in both generations at 50 mg/kg. Maternal and paternal general toxicity: reduced weight gain in the high-dose group Reproductive toxicity observed in parental animals: reduced litter size in high-dose group Reproductive toxicity observed in offspring: reduced survival and weight gain in high-dose group. Sporadic occurrences at mid-dose level.
NOEL	:	50 mg/kg (P generation)
NOEL	:	5 mg/kg (F1 generation)
NOEL	:	5 mg/kg (F2 generation)
Method	:	EPA/TSCA; parental rats and their offspring were observed, weighed, and examined for treatment-related effects.
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	
Source	:	
Reference	:	Robinson, E.C. and Schroeder, R.E., Reproductive and Developmental Toxicity Studies of a Linear Alkylbenzene Mixture in Rats; Fund. Appl. Toxicol 18, 549-556 (1992). (29)
Flag	:	Cited in SIAR

5.9 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	oral
Exposure period	:	days 6 through 15 of gestation
Doses	:	0, 125, 500, and 2000 mg/kg/day, administered in corn oil
Result	:	Maternal weight gain was reduced in all treatment groups and these differences were statistically significant at the mid- and high-dose groups. Food consumption was also lower in these groups. Ossification variations and delayed ossification were significantly increased at the high dose level and were increased above control at the mid-dose level. Maternal general toxicity: reduced weight gain, primarily in mid- and high dose groups Pregnancy and litter data: no treatment related effects Foetal data: skeletal (ossification) changes in mid- and high-dose groups
NOEL	:	125 mg/kg (maternal)
NOEL	:	125 mg/kg (offspring)
Method	:	EPA/TSCA; pregnant rats received daily dose of 0, 125, 500, and 2000 mg/kg of Alkylate 215 administered in corn oil on days 6 through 15 of gestation. Dams and fetuses were observed for treatment related effects.
Year	:	

GPL	:	yes
Test Substance	:	Alkylate 215 (<1% C_9, 16% C_{10}, 43% C_{11}, 40% C_{12}, 1% C_{13}, <1% C_{14})
Remarks	:	The fetal findings were considered evidence of a fetotoxic effect
Source	:	
Reference	:	Robinson, E.C. and Schroeder, R.E.; Reproductive and Developmental Toxicity Studies of a Linear Alkylbenzene Mixture in Rats; Fund. Appl. Toxicol 18, 549-556 (1992). (29)
Flag	:	Cited in SIAR
Species	:	rat
Sex	:	female
Strain	:	Sprague-Dawley
Route of admin.	:	oral
Exposure period	:	on days 6 through 15 of gestation
Doses	:	0, 125, 500, and 2000 mg/kg/day, administered in corn oil
Result	:	Maternal weight gain was reduced in all groups and this difference was statistically significant at the mid- and high-dose groups. Food consumption was also reduced in these groups. Ossification variations were increased in the mid- and high-dose groups. Retardation in kidney development (distended renal pelvis and distended tortuous ureter) was also present at the high-dose level. Maternal general toxicity: reduced weight gain primarily in the mid-and high dose groups Pregnancy and litter data: no treatment related effects Foetal data: skeletal (ossification) changes in the mid- and high-dose group. Soft tissue (kidney) changes in the high-dose group.
NOEL	:	maternal animals: 125 mg/kg
NOEL	:	offspring: 125 mg/kg
Method	:	EPA/TSCA; pregnant rats received daily dose of 0, 125, 500, and 2000 mg/kg of Alkylate 230 administered in corn oil on days 6 through 15 of gestation. Dams and fetuses were observed for treatment related effects.
Year	:	
GPL	:	yes
Test Substance	:	Alkylate 230 (1% C_{10}, 2% C_{11}, 16% C_{12}, 50% C_{13}, 30% C_{14}, 1% C_{15})
Remarks	:	Cited in SIAR
Source	:	
Reference	:	Monsanto Report BD-84-315 (9)
Flag	:	

5.10 OTHER RELEVANT INFORMATION

(1) Council of LAB/LAS Environmental Research. 1990. "Alkylbenzenes Summary of Safety Assessment", September, 1990.

(2) CSL Report No. 6589-67

(3) Dixie Services, Inc. 1991. Report No. 54142, Dec. 4, 1991

(4) Gledhill,W.E., Saeger, V.W. and Trehy, M.L. 1991. An Aquatic Environmental Safety Assessment of Linear Alkylbenzene. Env. Tox. and Chem. 10:169 - 178

(5) Iversen, O.H. 1990. Turmorigenesis and Carcinogenesis studies of a number of insulation oils and fluids and hairless and SENCAR mice with special reference to skin tumors and malignant lymphomas. APMIS Suppl. 13, Vol. 98, pp 3-60.

(6) Monsanto Report ABC-27560

(7) Monsanto Report ABC-27561

(8) Monsanto Report BD-84-277

(9) Monsanto Report BD-84-315

(10) Monsanto Report BT-65-2

(11) Monsanto Report BT-65-3

(12) Monsanto Report BT-65-4

(13) Monsanto Report HL-84-290

(14) Monsanto Report ML-80-58

(15) Monsanto Report ML-80-71

(16) Monsanto Report ML-80-71A

(17) Monsanto Report ML-82-1

(18) Monsanto Report MO-810174. Acute Toxicity of Alkylate 215 to the Midge (*Paratanytarsus parthenogenetica*).

(19) Monsanto Report SH-81-1

(20) Monsanto Study ES-81-SS-41

(21) Monsanto, unpublished

(22) Robinson, E.C. and Nair, R.S. 1992. The genotoxic potential of linear alkylbenzene mixtures in a short-term test battery. Fund. Appl. Toxicol 18, 540-548. Based on Monsanto Report DA-79-367

(23) RT LAB No. 871188

(24) RT LAB No. 925620

(25) RT LAB No. 925621

(26) S.A. Report 202093

(27) Vista Analytical Report

(28) Werner, F. and R.A. Kimerle. 1982. Uptake and distribution of C_{12} alkylbenzene in bluegill (*Lepomis macrochirus*). Environ. Toxicol. Chem. 1:143-6.

(29) Robinson, E.C. and Schroeder, R.E. 1997. Reproductive and Developmental Toxicity Studies of a Linear Alkylbenzene Mixture in Rats. Fund. Appl. Toxicol 18, 549-556.

(30) Unpublished, U.S. EPA model run using EPIWIN (SRC) version 3.10, May 2002.

TABLE 1

COMMERCIAL LINEAR ALKYLBENZENES

TYPICAL PRODUCT COMPOSITION

Product	Component Percentage							
	C9	**C10**	**C11**	**C12**	**C13**	**C14**	**C15**	**C16**
Alkylate 215	<1	16	43	40	1	<1	-	-
Alkylate 225	<1	7	25	48	19	1	-	-
Alkylate 229	<1	1.1	7.6	36.4	45.2	9.6	<1	-
Alkylate 230	-	1	2	16	50	30	1	-
Nalkylene 500	1	21	39	31	7	<1	-	-
Nalkylene 500L	<1	20	44	31	5	<1	-	-
Nalkylene 550L	<1	14	30	29	20	7	<1	-
Nalkylene 575L	<1	9	17	28	30	15	<1	-
Nalkylene 580L	-	-	<1	26	74	<1	-	-
Nalkylene 600	<1	<1	1	23	50	25	<1	-
Nalkylene 600L	<1	<1	1	23	50	25	<1	-