Section 1 – Chemical Product and Company Identification

MSDS Name: Phenyllithium in DBE

Chemical Family: Aryl Lithium

Molecular Formula: C_6H_5Li

Use of the substance: Experimental use only

Company: Optima Chemicals Group, LLC
200 Willacoochee Hwy.
Douglas, Georgia 31535
Telephone (912) 384-5101 FAX (912) 384-6330
Emergencies: Telephone (912) 384-5101

Section 2 – Hazards Identification

Hazards:

Flammable liquid, corrosive to eyes (may cause blindness), skin , nose, and throat. Contains benzene, which is a chemical known in the state of California to cause cancer.

Precautions:

Keep away from sources of ignition, water, air, acids and oxidizing materials, keep container tightly closed and protect against leaks and physical damage. Wear chemical splash goggles with a face shield, rubber gloves and rubber clothing. wash thoroughly after handling, do not get in eyes or on skin or clothing. Use in a closed system under insert atmosphere of argon or nitrogen.

NFPA Rating: Health: 3 Flammability: 4 Reactivity: 2 Special: W

In case of fire do not use water or carbon dioxide. Use dry chemical.

Section 3 – Composition, Information on Ingredients

CAS #	Chemical Name	Wt.%
591-51-5	Phenyllithium	17 -24
142-96-1	Dibutyl ether (DBE)	75-81
92-52-4	Biphenyl	<2

Section 4 – First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, lifting upper and lower lids intermittently. Seek medical attention.

Skin: Quickly wipe off as much as possible, then immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and/or shoes. Thoroughly wash with soap and water, and seek medical attention.

Ingestion: Quickly wipe material from the mouth, and rinse mouth out with plenty of water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Seek medical attention.

Inhalation: Remove from exposure, to fresh air immediately. If not breathing give artificial respiration, and seek medical attention.

Notes to Medical Doctor: This product is corrosive to eyes, skin, respiratory and gastrointestinal tracts. Treatment should first remove as much material as possible as quickly as possible, then flush with very large quantities of water. Ingestion presents a singular problem as emesis may produce esophageal damage and/or aspiration damage. Consideration should be given to gastric lavage with a large diameter tube for removal of material and then dilution with large amounts of water. Esophagoscopy may be of assistance in this procedure and to assess extent of damage. Treatment is otherwise symptomatic and supportive.

Section 5 – Fire Fighting Measures

Flammable Limits: Not avail

General Hazard: Flammable liquid. Reacts violently with water to give off flammable gases and corrosive dust.

Fire Extinguishing Agents Recommended: Do not use water or CO2, use a dry chemical powder.

Hazardous Combustion Products: Carbon dioxide, carbon monoxide, lithium hydroxide.

Special Fire fighting Procedures: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.

Autoignition temperature: Not applicable.

Properties contributing to flammability: Water reactivity of product, and volatility of solvents.

Flashpoint: 8 degrees C, THF -14.4 degrees C, Cumene 36 degrees C

Sensitivity to Static Discharge: Yes

Sensitivity to Impact: None

Section 6 – Accidental Release Measures

Remove all sources of ignition. Cover spill with dry extinguishant. Contain spill with absorbent. Transfer to approved transport container and clean up spillage with an absorbent. Dispose of waste according to local and Federal laws and regulations. Before cleanup measures begin, review the entire MSDS with particular attention to Section 3, and Section 8.

Section 7 - Handling and Storage

Handling: Do not get in eyes, on skin or clothing. Do not breathe vapors or mist. Use in a closed system under argon or nitrogen.

Storage: Store in cool, dry place. Store in tightly closed container. Keep away from sources of ignition, water, air, and oxidizing materials.

Section 8 – Exposure Controls, Personal Protection

Exposure Limits:

Chemical	PEL (OSHA)	TWA (ACGIH)	STEL/Ceiling (OSHA)	STEL/Ceiling (ACGIH)
Cumene	50 ppm	50 ppm	NA	NA
THF	200 ppm	50 ppm	NA	200 ppm

The IDLH for THF is 2,000 ppm

Engineering Controls: Use in closed system under argon or nitrogen. If personal contact can occur, use local exhaust ventilation (explosion proof), to keep airborne concentrations low.

Eyes and Face: Wear splash goggles with a face shield.

Skin: Chemical resistant gloves and clothing.

Respiratory: When engineering controls are not adequate, wear a NIOSH/MSHA respirator approved for protection against organic vapors and mists.

Work Hygienic Practices: Quick-drench eyewash and safety shower.

Section 9 – Physical and Chemical Properties

Appearance and Odor: Yellow to Amber, gasoline like odor.

Melting Point: -95ºC DBE Boiling Point: 142ºC DBE

Flash Point, Closed Cup (ASTM D3278-82): 142ºC (DBE)

Vapor Pressure: Not Available *Vapor Density Air = 1 : 1*

pH @ 25ºC, 1% soln.: Not Applicable Percent Volatile: 76-85

Water Solubility: reacts to water Evaporation Rate: Not available

Flammable Limits: Not Available Molecular Weight: 84.05

Autoignition Temperature: Not available Viscosity: Not available

Decomposition Temperature: Not available Explosive Properties: Not explosive

Oxidizing Properties: Not an oxidizer

Section 10 – Stability and Reactivity

Stability: Stable

Incompatibility: Heat, fire, air, water, and oxidizing chemicals.

Hazardous Polymerization: Does not polymerize

Hazardous Decomposition Products: Lithium hydroxide, lithium oxide, magnesium oxide and methane gas.

Conditions to Avoid: Heat, exposure to air or water, sparks, or flames.

Section 11 – Toxicological Information

Eyes: No data available for the product. Corrosive.

Skin: No data available for the product. Corrosive. Cumene: Dermal LD_{50} = 12300 uL/kg (rabbit) [RTECS]

Ingestion: No data available for the product. Corrosive. Cumene: Oral LD_{50} = 1400 mg/kg (rat) [RTECS], THF: Oral LD_{50} = 1650 mg/kg (rat) [RTECS]

Inhalation: No data available for the product. Corrosive. Cumene: LC_{50} = 10gm/cu.m/7H (mouse) [RTECS}, THF: LC_{50} = 21,000 ppm, 3 hr., (rat) [RTECS]

Acute Effects from Overexposure: This product is corrosive to the eyes (may cause blindness), skin, respiratory and gastrointestinal tracts. Inhalation of vapors may cause dizziness, nausea, anesthesia, numbness, burning sensation and motor weakness in fingers and toes, incoordination, and headache. Low viscosity material – if swallowed may enter the lungs and cause lung damage.

Chronic Effects from Overexposure: No data available for the product. THF: Repeated or prolonged exposure may cause signs of central nervous system depression and respiratory irritation.

Sensitization: No data available.

Carcinogenicity: Not listed by OSHA, EH40, or IARC. THF is listed as a substance that is reasonably anticipated to be a carcinogen by NTP. ACGIH lists THF as a Category A3 – a confirmed animal carcinogen with unknown relevance to humans.

Mutagenicity: No data available for the product. THF gave negative results in bacterial mutagenicity tests with and without metabolic activation.

Reproductive Toxicity: No data available for the product. One animal study suggests that THF does not cause effects at doses which are not maternally toxic.

Section 12 – Ecological Information

Ecotoxicological Information: No data available for the product. Cumene: 48 hr LC_{50} = 0.6 ppm (Daphnia magna), 96 hr LC_{50} = 6.32 mg/l/96 (Fathead minnow) [Handbook Env. Data on Org. Chem. 4^{th} Ed]. THF 48 hr LC_{50} = 2820; 2930 mg/l (orfe), 96 hr LC_{50} = 2160 mg/l (fathead minnow) [Handbook Env. Data on Org. Chem. 4^{th} Ed].

Chemical Fate Information: No data available. The product reacts with water to form methane and lithium hydroxide.

Cumene: Readily volatilized from surface water and soil and is expected to have low to moderate environmental persistence. Cumene which is not volatilized and degraded is expected to be biodegraded or adsorbed to soil particles.

THF: Expected to volatilize from both water and soil and leach into groundwater. It will not photodegrade or adsorb to sediment. Limited evidence suggests it may biodegrade. Based on a relatively low Kow (0.47), it is expected to bioconcentrate.

Section 13 – Disposal Considerations

Dispose of in accordance with federal, state, and local regulations.

Section 14 – Transport Information

Proper Shipping Name: Flammable liquid, corrosive, N.O.S. (methyllithium in cumene/tetrahydrofuran)

UN Number: UN2924

Classification: 3, Flammable liquid, (8, Corrosive)

Packing Group: PG ll

Labels: Flammable, Corrosive

Marine Pollutant: No

Custom Tariff Number: 2931.00.9160

PIH: Not designated Poison Inhalation Hazard by USDOT.

Section 15 – Regulatory Information

United States:

Section 311 Hazard Category (40CFR 370): Reactive, fire hazard, acute health hazard, chronic health hazard.

Section 313 Reportable Ingredients (40 CFR 372): Cumene is reportable.

Section 302 Extremely Hazardous Substances (40 CFR 355): Not listed.

CERCLA Hazardous Substance, RQ, (40 CFR 302.4): Cumene – 5,000 pounds, THF - 1,000 pounds.

TSCA Sec 12B Export Notification: Yes, due to THF.

TSCA Inventory Status (40 CFR 710): Listed

Canada:

WHMIS: Hazard Classification – UN 3394, Class B, Division 2 (Flammable liquid), Class B, Division 6 (Reactive Flammable Materials, Flammable gas on contact with water), Class E, (Corrosive).

Ingredient Disclosure List: Cumene and THF are listed.

Section 16 – Additional Information

Creation Date: 1/20/2010

This MSDS has been prepared to meet U.S. OSHA Hazard Communication Standard, 29 CFR 1910.1200, the Canada's Workplace Hazardous Materials Information System (WHMIS) requirements, and the Global Harmonization System (GHS).

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