Section 1 – Chemical Product and Company Identification

MSDS Name: t-Butyllithium in Heptane

Chemical Family: Alkyllithium

Molecular Formula: C_4H_9Li

Synonyms: 2-Lithio-2-Methylpropane

Use of the substance: Industrial manufacturing

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:

Pyrophoric liquid. Can catch fire if exposed to air. Reacts violently with water to give off flammable gases and corrosive dusts.

Handle under nitrogen or other inert gas.

Corrosive - Causes severe skin burns, eye damage, and is extremely destructive to tissue of the mucous membranes and upper respiratory tract. Can catch fire on contact with body moisture. Inhalation of vapors may cause dizziness, nausea, anesthesia, numbness, motor weakness in fingers and toes, incoordination, and headache.

NFPA Rating: Health: 3 Flammability: 4 Reactivity: 3 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.%
594-19-4	tertiary-Butyllithium	15-30
64742-49-0	Heptanes	70-85

Section 4 – First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, lifting upper and lower lids. 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. 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. Consideration should be given to careful endoscopy as stomach or esophageal burns, perforations or strictures may occur. Careful gastric lavage with an endotracheal tube in place should be considered. Treatment is otherwise symptomatic and supportive.

Section 5 – Fire Fighting Measures

Flammable Limits: Heptane- Upper: 6.7% Lower: 1.1%

General Hazard: Pyrophoric liquid. Air and oxygen sensitive. Flammable liquid.

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: Heptane: -7.8 degrees C

Sensitivity to Static Discharge: Yes

Sensitivity to Impact: Not applicable

Section 6 – Accidental Release Measures

Remove all sources of ignition. Spilled material can catch fire spontaneously on contact with air, moisture, acids or oxidizing materials. 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: Keep away from water, air, and oxidizing materials. 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: n-Pentane - PEL (OSHA) - 500 ppm, TWA (ACGIH) – 400 ppm, STEL/Ceiling (OSHA) – None, STEL/Ceiling (ACGIH) – 500 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: Clear white to pale yellow, gasoline like odor.

Melting Point: Not available Boiling Point: Heptane, 94-99 degrees C

Flash Point: Heptane, -7.8 degrees C

Vapor Pressure: Heptane, 44.6 mmHg

Vapor Density: Not available

pH: Not available

Specific Gravity: 0.7 g/ml @ 20 degrees C

Percent Volatile: 70-90%

Water Solubility: Insoluble, reacts violently

Evaporation Rate: Heptane, 5.0

Flammable Limits: Heptane, Upper 6.7%
Lower 1.1%

Molecular Weight: 64.06

Autoignition Temperature: Not applicable

Viscosity: Not available

Decomposition Temperature: Not available

Explosive Properties: Not explosive

Oxidizing Properties: Not an oxidizer

Section 10 – Stability and Reactivity

Stability: Stable at room temperature

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

Hazardous Polymerization: Does not polymerize

Hazardous Decomposition Products: Carbon monoxide, carbon dioxide, lithium hydroxide, lithium hydride, butane gas.

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

Section 11 – Toxicological Information

Eyes: No data available. Corrosive.

Skin: No data available. Corrosive.

Ingestion: No data available. Corrosive.

Inhalation: No data available. Corrosive. n-Heptane: LC50 = 103 gm/m^3/4H (rat)

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.

Chronic Effects from Overexposure: No data available.

Sensitization: No data available.

Carcinogenicity: Not listed by NTP, OSHA, EH40. IARC, or ACGIH.

Mutagenicity: No data available.

Reproductive Toxicity: No data available.

Section 12 – Ecological Information

Ecotoxicological Information: No data available for product. n-Heptane: 24h LC_{50} = 4 mg/L (goldfish) [Env. Data on Org. Chem., 4th ed], 24-96h LC_{50} = 4924 mg/L (mosquito fish) [Env. Data on Org. Chem, 4th ed], 48h EC_{50} = 1.5 mg/L (daphnia magna) [Env. Data on Org. Chem, 4th ed].

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

n-Heptane will readily volatize from both soil and water. If released to water the product will float. The product is insoluble in water. If released to soil it will evaporate at a rapid rate. The product is poorly absorbed onto soils or sediments. The product is expected to be readily biodegradable. Photochemical degradation in air will proceed at a moderate rate. BOD_5 = 55% of ThOD. Heptane is not expected to bioaccumulate.

Section 13 – Disposal Considerations

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

Section 14 – Transport Information

DOT Shipping: Organometallic substance, liquid, pyrophoric, water-reactive (tert-butyllithium, hydrocarbon solution), 4, Spontaneously Combustible, Dangerous When Wet, UN3394, PG I

Labels: Spontaneously Combustible, Dangerous When Wet

Marine Pollutant: No

Custom Tariff Number: 2931.00.9060

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): No reporting requirements.

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

CERCLA Hazardous Substance, RQ, (40 CFR 302.4): Not listed.

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

TSCA Inventory Status (40 CFR 710): Listed

Canada:

WHMIS: Hazard Classification – UN 3394, Class B, Division 6 (Reactive Flammable Materials), Class E, (Corrosive), Ingredient Disclosure List: Heptane is listed.

Section 16 – Additional Information

Creation Date: 1/11/2010

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

This information is believed to be accurate and represents the best information currently available to Optima Chemical Group LLC. However, we make no warranty of merchantability, express or implied, with respect to such information and assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes.