

**SAFETY DATA SHEET**

**T-BUTYLLITHIUM IN HEPTANE**

**1. Identification of the Substance/Mixture and of the Company/Undertaking:**

- 1.1 **Product Identifier:** t-Butyllithium in Heptane
- 1.1.1 **Substances** Not applicable
- 1.1.2 **Mixture name:** t-Butyllithium in Heptane
- 1.2 **Relevant Identified Uses of the Substance or Mixture and Uses Advised Against:**  
 Industrial Manufacturing  
 Only to be supplied for industrial uses  
 For use only as a chemical intermediate under strictly controlled conditions
- 1.3 **Details of the Supplier of the Safety Data Sheet**

**North America**  
 FMC Corporation  
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 Charlotte, NC 28208  
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Email: [lithium.info@fmc.com](mailto:lithium.info@fmc.com)  
 Web: [www.fmclithium.com](http://www.fmclithium.com)

1.4 **Emergency Telephone Number:**

**North America**  
**CHEMTREC:** +1.800.424.9300  
 +1.703.527.3887  
**Plant:** +1.704.629.5361  
**Medical:** +1.303.595.9048

**Europe**  
**24 hr Specialist advice number:**  
**CHEMTREC:** +44 870 8200418

**Asia Pacific**  
 Phone: +86.21.2067.5888

**2. Hazards Identification**

- 2.1 **Classification of the Mixture:**  
**2.1.1 GHS Classification [EC Regulation No 1272/2008 and US OSHA regulations]**  
 Pyrophoric liquid; Category 1  
 Water reactive; Category 1  
 Flammable liquid; Category 2  
 Skin corrosive; Category 1B  
 Eye damage; Category 1  
 Aspiration toxicity; Category 1  
 Specific target organ systemic toxicity – SE Category 3  
 Hazardous to the aquatic environment – Chronic;  
 Category 2
- 2.2.2 EC: Classification according to 67/548/EEC or 1999/45/EC [DSD/DPD]**  
 F, R14/15, R17; C, R34; Xn, R65, R67; N R51/53

2.2 **Label Elements:**  
 2.2.3 **Hazard Pictograms:**





**2.2.4 Signal Word:**

**Hazard Statement(s):**

Danger  
 Catches fire spontaneously if exposed to air. H250  
 In contact with water releases flammable gases, which may ignite spontaneously. H260  
 Causes severe skin burns and eye damage. H314  
 Highly flammable liquid and vapour. H225  
 May be fatal if swallowed and enters airways. H304  
 May cause drowsiness or dizziness. H336  
 Suspected of damaging fertility. H361f  
 May cause damage to organs through prolonged or repeated exposure. H373  
 Toxic to aquatic life with long lasting effects; H411

**Precautionary Statement(s):**

Handle under inert gas. Protect from moisture. P231 + P232  
 Do not allow contact with air. P222  
 Keep away from any possible contact with water, because of violent reaction and possible flash fire. P223  
 Wear protective gloves/protective clothing/eye protection/ face protection. P280  
 In case of fire: Use dry chemical for extinction. P370 + P378  
 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting. P301 + P330 + P331  
 IF ON SKIN (or hair): Remove / Take off immediately all contaminated clothing. Rinse skin with water / shower. P303 + P361 + P353  
 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P305 + P351 + P338  
 Immediately call a POISON Center or doctor/physician. P310

**Additional Precautionary Phrases:**

Keep away from heat/sparks/open flames/hot surfaces. – No smoking. P210  
 Keep away from any possible contact with water, because of violent reaction and possible flash fire. P223  
 Ground/bond container and receiving equipment. P240  
 Use explosion-proof electrical/ventilating/lighting/.../equipment. P241  
 Use only non-sparking tools. P242  
 Take precautionary measures against static discharge. P243  
 Do not breathe dust/fume/gas/mist/vapours/spray. P260  
 Wash hands thoroughly after handling. P264  
 Use only outdoors or in a well-ventilated area. P271  
 If INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. P304 + P340  
 Wash contaminated clothing before reuse. P363  
 Store in a dry place. Store in a closed container. P402 + P404  
 Store in a well-ventilated place. Keep cool. P403 + P235  
 Store locked up. P405  
 Dispose of contents/ container to an approved waste disposal plant. P501

**2.3 Other Hazards**

Reacts violently with water EUH014

**3. Composition / Information on Ingredients**

**3.1 Substances**

Not applicable.

**3.2 Mixtures**

**3.1.1 GHS Classification [EC: Regulation No 1272/2008; US: OSHA regulations]**

<u>Chemical Name</u>	<u>CAS #</u>	<u>EC No</u>	<u>EC Index No</u>	<u>REACH Reg No</u>	<u>Wt.%</u>	<u>Classification, Hazard Statement Codes</u>
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t-Butyllithium	594-19-4	209-831-5	None	None	10 - 31	Pyr. Liq. 1 Water-react. 1 Skin Corr. 1B	H250 H260 H314
Heptanes	64742-49-0	927-510-4 (Provisional.)	None	01-2119475515-33-****	69 – 90	Flam. Liq. 2 Skin Irrit. 2 Asp. Tox. 1 STOT SE 3 Aquatic chronic 2	H225 H315 H304 H336 H411

**3.1.2 EC: Classification according to 67/548/EEC or 1999/45/EC [DSD/DPD]**

Chemical Name	CAS #	EC No	Wt.%	Symbols	R-phrases
t-Butyllithium	594-19-4	209-831-5	10 - 31	F C	R14/15, R17; R34;
Heptanes	64742-49-0	927-510-4 (Provisional.)	69 – 90	F; Xn; Xi;  N;	R11 R65 R38 R67 R51/53

(See Section 16 for R-phrases text)

## 4. First Aid Measures

### 4.1 Description of First Aid Measures

- EYES:** Immediately flush with water for at least 15 minutes, lifting the upper and lower eyelids intermittently. See a medical doctor or ophthalmologist immediately.
- SKIN:** Immediately flush with plenty of water while removing contaminated clothing and/or shoes, and thoroughly wash with soap and water. Obtain immediate medical attention. Contact a medical doctor if necessary.
- INGESTION:** Quickly wipe material from the mouth and rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. See a medical doctor immediately.
- INHALATION:** Remove to fresh air. If breathing discomfort occurs and persists, see a medical doctor. If breathing has stopped, give artificial respiration and see a medical doctor immediately.

### 4.2 Most important symptoms and effects, both acute and delayed

Symptoms of over-exposure will typically be a result of the corrosive nature of the substance with discomfort to skin and if swallowed, local effects with discomfort to the mouth and GI tract. Inhalation of solvent vapours may lead to dizziness and impairment of normal functions.

### 4.3 Indication of any immediate medical attention and special treatment needed.

**Notes to medical doctor:**

Product is highly alkaline and is corrosive to the eyes, skin and mucous membranes. 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. Observation may be warranted. Treatment is controlled removal of exposure followed by symptomatic and supportive care.

## 5. Fire-Fighting Measures

- 5.1 Extinguishing media** DO NOT USE WATER OR CARBON DIOXIDE. Use dry chemical.
- 5.2 Special hazards arising from the substance or mixture**
- Hazardous combustion products** Lithium hydroxide, carbon monoxide, carbon dioxide.
- General Hazard** Pyrophoric. Water reactive. Flammable liquid.
- Properties contributing to**
- Flammability** Water reactivity (pyrophoricity) of product, and volatility of solvents.
- Flashpoint** Not applicable for formulation. The flashpoint of heptane is –7.8 C°
- Flammable limits in air** Not applicable for formulation. For heptanes (approximate): Upper: 6.7 wt% Lower: 1.1 wt%
- Auto ignition temperature** Not applicable. t-Butyllithium in heptanes is pyrophoric at room temperature and 50% humidity.
- Sensitivity to static discharge** Yes
- Sensitivity to static impact** Not applicable
- 5.3 Advice for fire-fighters**

Wear full protective clothing and self-contained breathing apparatus (SCBA) approved for fire fighting. This is necessary to protect against the hazards of heat, products of combustion and oxygen deficiency. Do not breathe smoke, gases or vapors generated.

**COMMENTS:**

(See Section 10, Stability and Reactivity)

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**6. Accidental Release Measures**

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**6.1 Personal precautions, protective equipment and emergency procedures**

Before cleanup measures begin, review the entire SDS with particular attention to Section 2, Hazards Identification; and Section 8, Exposure Controls/Personal Protection. Remove all sources of ignition. Spilled material can catch fire spontaneously on contact with air, moisture, acids or oxidizing materials.

**6.2 Environmental precautions**

Contain spill. Do not wash into drains. Dispose of at qualified waste disposal facility.

**6.3 Methods and material for containment and cleaning up**

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. DO NOT USE WATER OR CARBON DIOXIDE. Contain spill with absorbant. Expose to air until solvent has dissipated. Sweep up and place in approved transport container. Dispose of waste according to local and Federal laws and regulations.

**6.4 Reference to other sections**

Before cleanup measures begin, review the entire SDS with particular attention to Section 2, Hazards Identification; and Section 8, Exposure Controls/Personal Protection.

**6.5 Additional information**

Not specified.

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**7. Handling and Storage**

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**7.1 Precautions for safe handling**

KEEP AWAY FROM WATER, AIR AND OXIDIZING MATERIALS. Wear a face shield with either chemical splash goggles or safety glasses. Use in a closed system under argon or nitrogen.

**7.2 Conditions for safe storage, including any incompatibilities**

Keep away from heat, sparks and flame. Store away from other flammable or combustible materials. Protect storage container from leaks and physical damage.

**7.3 Specific end use(s)**

For use only as a chemical intermediate under strictly controlled conditions

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**8. Exposure Controls / Personal Protection**

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**8.1 Control parameters**

**DNEL**

**Hydrocarbons, C7, n-alkanes, isoalkanes, cyclic; Heptanes**

Long-term exposure, systemic, inhalation 2085 mg/m<sup>3</sup>  
 Long-term exposure, systemic, dermal 300 mg/kg/day

**PNEC**

**Heptanes**

No details published

**EXPOSURE LIMITS**

Chemical Name	EU		EH40 (UK WEL)		USA (ACGIH)		USA (OSHA)	
	TWA	STEL	TWA	STEL	TWA	STEL/Ceiling	PEL	STEL/Ceiling
n-Heptane	none*		500 ppm	1500 ppm	400 ppm	500 ppm	500 ppm	

**8.2 Exposure controls**  
Refer to appropriate Exposure Scenarios

**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 below exposure limits.

**Personal protective equipment**

**Eyes and Face:** Face shield with either chemical splash goggles or safety glasses.

**Respiratory:** Wear a respirator approved for protection against organic vapours and mists when adequate ventilation is not available  
US: NIOSH or MSHA approved  
Europe: CEN Class A type

**Protective Clothing:** **Gloves:** Nitrile (typical permeation breakthrough time >480 minutes)  
These glove recommendations should not be used as the absolute basis for glove selection. Actual in-use conditions may vary glove performance from the controlled conditions of laboratory tests. Factors such as concentration and temperature, glove thickness and glove reuse, may affect performance. Other glove requirements, such as length, dexterity, cut, abrasion, puncture and snag resistance, or glove grip need to be considered in making your final selection. For flammable products, the recommended gloves provide chemical but not fire protection

**Other:** Flame resistant aramid fibre (Nomex® or equivalent. Nomex® is a registered trademark of E. I. du Pont de Nemours and Company

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

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## 9. Physical and Chemical Properties

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**9.1 Information on basic physical and chemical properties**

<b>Appearance:</b>	Clear, water-white to pale yellow liquid
<b>Odor:</b>	Gasoline-like
<b>Odor threshold:</b>	Not available
<b>pH:</b>	Reacts violently with water giving mixture with pH >12
<b>Melting point:</b>	Not available
<b>Boiling point:</b>	94-99 C° (heptane, approximate)
<b>Flash point:</b>	Not applicable for formulation. The flashpoint of heptane is – 7.8 C°
<b>Evaporation rate(butyl acetate = 1):</b>	5.0 (heptane, approximate)
<b>Flammability:</b>	Pyrophoric and water reactive material in flammable liquid solvent
<b>Flammable limits:</b>	Not applicable for formulation. For heptane (approximate): Upper: 6.7 wt% Lower: 1.1 wt%
<b>Vapor pressure:</b>	44.6 mmHg @ 20 °C (heptane, estimate)
<b>Vapor density (air = 1):</b>	Not available
<b>Specific gravity:</b>	0.7 g/ml @ 20 °C
<b>Solubility in water:</b>	Reacts violently with water
<b>Partition coefficient n-octanol/ water:</b>	Not available
<b>Autoignition temperature:</b>	Not applicable. t-Butyllithium in heptanes is pyrophoric at room temperature and 50% humidity.
<b>Decomposition temperature:</b>	Not available
<b>Viscosity:</b>	Not available
<b>Explosive properties:</b>	Not explosive
<b>Oxidizing properties:</b>	Not an oxidizer

**9.2 Other information**

<b>Self-reactive properties</b>	Does not meet classification criteria.
<b>Pyrophoric properties</b>	t-Butyllithium in heptanes is pyrophoric.
<b>Self-heating properties</b>	Does not meet classification criteria.
<b>Water reactive properties</b>	t-Butyllithium in heptanes is a packing group I water reactive.
<b>Corrosive to metals</b>	Does not meet classification criteria.
<b>Molecular weight:</b>	64.06

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## 10. Stability and Reactivity

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10.1 <b><u>Reactivity</u></b>	Reactive with water and damp air
10.2 <b><u>Chemical stability</u></b>	Stable if kept away from air and moisture. Will slowly degrade to lithium hydride and butene. Rate of degradation is dependent on temperature.
10.3 <b><u>Possibility of hazardous reaction</u></b>	Reaction with water, air, oxidizers, acids to form lithium hydroxide, butane gas.
10.4 <b><u>Conditions to avoid</u></b>	Open air. Heat, sparks or flames
10.5 <b><u>Incompatible materials</u></b>	Water, damp air, carbon dioxide. Mixtures of butyllithium with organic compounds containing oxygen, or with halogenated organic compounds can react, generating dangerous quantities of heat and gas.
10.6 <b><u>Hazardous decomposition products</u></b>	None

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## 11. Toxicological Information

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### 11.1 **Information on toxicological effects**

The mixture has not been tested, but properties can be predicted based on the properties of the two components

(a) acute toxicity	t-Butyllithium: Corrosive Heptanes: Oral LD <sub>50</sub> >5840 mg/kg Inhalation LC <sub>50</sub> >23300 mg/m <sup>3</sup> (rat, 4 hr)
(b) skin corrosion/irritation	Classified as corrosive on the basis of butyllithium.
(c) serious eye damage/irritation	Classified as corrosive on the basis of butyllithium.
(d) respiratory/skin sensitisation	No components are considered to be potential sensitizing agents.
(e) germ cell mutagenicity	None of the components considered to be mutagenic.
(f) carcinogenicity	None on the components considered to be carcinogenic
(g) reproductive toxicity	Classified as not a reproductive toxin based on butyllithium and heptanes.
(h) STOT-single exposure	Heptanes may cause drowsiness.
(i) STOT-repeated exposure	Classified as not causing organ damage based on butyllithium and heptanes.
(j) aspiration hazard	Heptanes may be fatal if swallowed and enters airways

The component heptanes, has been extensively tested for REACH registration. t-Butyllithium has been less extensively tested in view of the corrosivity and reactivity and in view of limited uses as intermediate.

#### **Acute Effects From Overexposure:**

No data available for the formulation. This product contains an alkyl lithium compound which is extremely reactive and corrosive to the skin, eyes (may cause blindness), nose, throat and stomach. 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 product.

Heptane: Prolonged contact with heptane may cause defatting of the skin and skin irritation.

#### **Carcinogenicity Listings**

Eh40: Not listed.  
IARC: Not listed.  
NTP: Not listed.  
OSHA: Not considered a carcinogen under OSHA.  
ACGIH: Not listed.

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## 12. Ecological Information

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### 12.1 **Toxicity:**

The mixture has not been tested, but properties can be predicted based on the properties of the components.

The mixture is predicted to be toxic to aquatic organisms based on cyclohexane

Butyllithium (note this reacts in water and data derived for other lithium salts)

Fish 96h LC<sub>50</sub> 109 mg/L

Daphnia 48h EC<sub>50</sub> 29 mg/L

Algae 96h IC<sub>50</sub> 3.4 mg/L

n-Heptane:

Fish 96h LC<sub>50</sub> : not toxic within limits of water solubility

Daphnia 48h EC<sub>50</sub> : not toxic within limits of water solubility

Algae 96h IC<sub>50</sub> : not toxic within limits of water solubility

## 12.2 Persistence and degradability

t-Butyllithium: t-Butyllithium reacts violently with water to form butane and lithium hydroxide.

Heptane: n-Heptane will readily volatilize 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<sub>5</sub> = 55% of ThOD. Heptane is not expected to bioaccumulate.

## 12.3 Bioaccumulative potential

Heptane is not expected to bioaccumulate

## 12.4 Mobility in soil

Solvents not expected to be mobile.

## 12.5 Results of PBT and vPvB assessment

A PBT and vPvB assessment has been undertaken for REACH and none of the components are considered to be of concern.

## 12.6 Other adverse effects

Due to the nature of the material and the specialist applications, this product is not considered to be a risk to the environment.

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## 13. Disposal Considerations

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### 13.1 Waste treatment methods

#### Disposal method:

Do not discharge to waste water systems.

Spent solvent may be sent for recovery or used as fuel if permitted under local regulations

Dispose of waste according to local and national laws and regulations.

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## 14. Transport Information

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### 14.1 UN Number

UN3394

### 14.2 UN proper shipping name (IMDG, ICAO, ADR, DOT)

Organometallic substance, liquid, pyrophoric, water-reactive (t-butyllithium, hydrocarbon solution)

### 14.3 Transport hazard class(es) (IMDG, ICAO, ADR, DOT)

4.2, Spontaneously combustible, (4.3, Dangerous When Wet)

### 14.4 Packing group (IMDG, ICAO, ADR, DOT)

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### 14.5 Environmental hazards

Marine pollutant due to presence of heptanes

### 14.6 Special precautions for user

None

### 14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

None

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## 15. Regulatory Information

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### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

#### EUROPEAN UNION:

#### German Wassergefährdungsklasse (water hazard class)

t-Butyllithium

not listed

heptanes

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**UNITED STATES:**

**Section 311 Hazard Category (40 CFR 370):**

Immediate (acute) health hazard, delayed (chronic) health hazard, fire hazard, reactive

**Section 313 Reportable Ingredients (40 CFR 372):**

This product does not contain a toxic chemical subject to the reporting requirements of Section 313 of Emergency Planning and Community Right-To-Know Act of 1986.

**Section 302 Extremely Hazardous Substances (40 CFR 355):**

Not listed

**CERCLA Hazardous Substance (40 CFR 302.4):**

Not listed

**TSCA Sec 12b Export Notification:**

This product is subject to TSCA 12(b) export notification requirements due to the presence of heptane.

**NFPA Rating:**

**Health: 3 Flammability: 4 Reactivity: 3 Special: ~~W~~**

**INTERNATIONAL INVENTORY STATUS:**

<b><u>Inventory/Country</u></b>	<b><u>Product Status</u></b>
EINECS (EU)	Listed
TSCA (US)	Listed
ECL (Korea)	Listed
DSL (Canada)	Listed

**15.2 Chemical Safety Assessment**

A Chemical Safety Assessment has not been carried out for t-butyllithium as it is registered for use as a strictly controlled intermediate.

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## 16. Other Information

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**European Union:**

Highly flammable.	R11
Irritating to skin.	R38
Reacts violently with water, liberating extremely flammable gases	R14/15
Spontaneously flammable in air	R17
Causes burns	R34
Harmful: may cause lung damage if swallowed	R65
Vapours may cause drowsiness and dizziness	R67
Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment	R51/53

**List of Abbreviations used in this SDS:**

PBT	Persistent, Bioaccumulative and Toxic
vPvB	very Persistent, very Bioaccumulative
PEC	Predicted environmental concentration
PNEC	Predicted no effect concentration
DNEL	Derived no effect level

**REVISION SUMMARY:** Revision # 1. Sections 7.1, 7.2, 8.2, 10.2 changed. Handling revised.

This SDS has been prepared to meet U. S. OSHA Hazard Communication Standard requirements.  
type 4

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