



## SAFETY DATA SHEET

## N-BUTYLLITHIUM IN HEXANES

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

- 1.1 **Product Identifier:** n-Butyllithium in hexanes  
1.1.1 **Substances** Not applicable  
1.1.2 **Mixture name:** n-Butyllithium in hexanes  
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  
2801 Yorkmont Road, Suite 300  
Charlotte, NC 28208  
Phone: +1.704.426.5300  
Fax: +1.704.426.5370  
1.888.lithium

**Europe**  
FMC Chemicals  
Commercial Road  
Bromborough, Merseyside  
CH62 3NL, England  
Phone: +44.151. 334.8085  
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**Asia Pacific**  
FMC Asia Innovation Center  
No 3 Building No. 4560  
Jinke Road  
Shanghai, China 201203  
T: +86.21.2067.5888

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

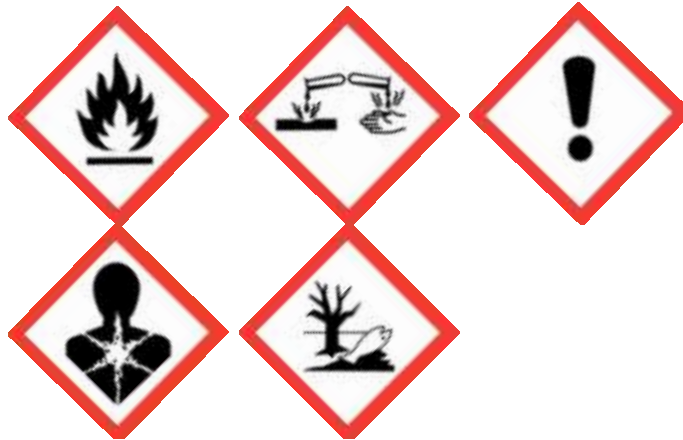
**Europe**  
24 hr Specialist advice number:  
CHEMTREC: +44 870 8200418

**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  
Reproductive toxicity; Category 2  
Specific target organ systemic toxicity – SE Category 3  
Specific target organ systemic toxicity – RE; Category 2  
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, R 65, R67, R48/20; Repr  
Cat. 3, R62; 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 Statement(s):**

Obtain special instructions before use.	P201
Do not handle until all safety precautions have been read and understood.	P202
Keep away from heat/sparks/open flames/hot surfaces. – No smoking.	P210
Ground/bond container and receiving equipment.	P240
Use explosion-proof electrical/ventilating/lighting/.../equipment.	P241
Use only non-sparkling 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
Use personal protective equipment as required.	P281
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
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### 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>
n-Butyllithium	109-72-8	203-698-7	None	01-2119494906-21-0001	10 - 31	Pyr. Liq. 1 H250 Water-react. 1 H260 Skin Corr. 1B H314 Flam. Liq. 2 H225
Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich *	None	925-292-5	None	01-2119474209-33-****	69 – 90	Skin Irrit. 2 H315 Asp. Tox. 1 H304 Repr. 2 H361f STOT SE 3 H336 STOT RE 2 H373 Aquatic chronic 2 H411

\* contains n-hexane, CAS# 110-54-3

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

<u>Chemical Name</u>	<u>CAS #</u>	<u>EC No</u>	<u>Wt. %</u>	<u>Symbols</u>	<u>R-phrases</u>
n-Butyllithium	109-72-8	203-698-7	10 - 31	F C	R14/15, R17; R34;
Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich *	None	925-292-5	69 – 90	F; Xi; Xn;  Repr.Cat.3; N;	R11 R38 R65, R67, R48/20 R62 R51-53

\* contains n-hexane, CAS# 110-54-3

(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.

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## 5. Fire-Fighting Measures

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- 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 hexane is  $-26\text{ C}^{\circ}$ .  
**Flammable limits in air** Not applicable for formulation. For hexane: Upper: 7.7 wt%  
Lower: 1.2 wt%  
**Auto ignition temperature** Not applicable. n-Butyllithium in hexanes 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**

Note that DNELs and PNECs have not been derived for butyllithium as it is a strictly controlled transported

intermediate

**DNEL Hexanes:**

**Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich**

Long-term exposure, systemic, inhalation 93 mg/m<sup>3</sup>  
 Long-term exposure, systemic, dermal 13 mg/kg/day

**Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich**

Long-term exposure, systemic, inhalation 93 mg/m<sup>3</sup>  
 Long-term exposure, systemic, dermal 13 mg/kg/day

**PNEC Hexanes:**

Not determined for the registration process  
 Estimated freshwater PNEC 0.05 mg/l using default factor 100.

**EXPOSURE LIMITS**

<u>Chemical Name</u>	<u>EU</u>		<u>EH40 (UK WEL)</u>		<u>USA (ACGIH)</u>		<u>USA (OSHA)</u>	
	<u>TWA</u>	<u>STEL</u>	<u>TWA</u>	<u>STEL</u>	<u>TWA</u>	<u>STEL/Ceiling</u>	<u>PEL</u>	<u>STEL/Ceiling</u>
n-Hexane	none*		20 ppm 72 mg/m <sup>3</sup>		50 ppm		50 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**

Quick-drench eyewash and safety shower.

**Practices:**

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**9. Physical and Chemical Properties**

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

**Appearance:** Clear, water-white to pale yellow liquid  
**Odor:** Gasoline-like  
**Odor threshold:** Not available  
**pH:** Reacts violently with water giving mixture with pH >12  
**Melting point:** Hexane: -95. C°  
**Boiling point:** Hexane: 62-69 °C  
**Flash point:** Not applicable for formulation. The flashpoint of hexane is -26 °C.  
**Evaporation rate(butyl acetate = 1):** 7.1 – 8.4 (hexane)  
**Flammability:** Pyrophoric and water reactive material in flammable liquid solvent

<b><u>Flammable limits:</u></b>	Not applicable for formulation. For hexane: Upper: 7.7 wt% Lower: 1.2 wt%
<b><u>Vapor pressure:</u></b>	Hexane: 5.6 psi @ 38 °C
<b><u>Vapor density (air = 1):</u></b>	(air=1): Approximately 3 (hexane)
<b><u>Specific gravity:</u></b>	0.7-0.8 g.ml @ 20°C (68°F)
<b><u>Solubility in water:</u></b>	Reacts violently with water
<b><u>Partition coefficient n-octanol/ water:</u></b>	Not available
<b><u>Autoignition temperature:</u></b>	Not applicable. n-Butyllithium in hexanes is pyrophoric at room temperature and 50% humidity.
<b><u>Decomposition temperature:</u></b>	Not available
<b><u>Viscosity:</u></b>	Not available
<b><u>Explosive properties:</u></b>	Not explosive
<b><u>Oxidizing properties:</u></b>	Not an oxidizer
<b>9.2 <u>Other information</u></b>	
<b><u>Self-reactive properties</u></b>	Does not meet classification criteria.
<b><u>Pyrophoric properties</u></b>	n-Butyllithium in hexane is pyrophoric.
<b><u>Self-heating properties</u></b>	Does not meet classification criteria.
<b><u>Water reactive properties</u></b>	n-Butyllithium in hexane is a packing group I water reactive.
<b><u>Corrosive to metals</u></b>	Does not meet classification criteria.
<b><u>Molecular weight:</u></b>	64.06

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## 10. Stability and Reactivity

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<b>10.1 <u>Reactivity</u></b>	Reactive with water and damp air
<b>10.2 <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.
<b>10.3 <u>Possibility of hazardous reaction</u></b>	Reaction with water, air, oxidizers, acids to form lithium hydroxide, butane gas.
<b>10.4 <u>Conditions to avoid</u></b>	Open air. Heat, sparks or flames
<b>10.5 <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.
<b>10.6 <u>Hazardous decomposition products</u></b>	Lithium hydride, butene

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## 11. Toxicological Information

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<b>11.1 <u>Information on toxicological effects</u></b>	
The mixture has not been tested, but properties can be predicted based on the properties of the two components	
(a) acute toxicity	Butyllithium: Corrosive n-Hexane discriminating oral dose > 2000 mg/kg n-Hexane acute inhalation toxicity > 17.6 mg/l (5000 ppm) n-Hexane acute dermal toxicity > 2000 mg/kg
(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	n-Hexane suspected of damaging fertility or the unborn child.
(h) STOT-single exposure	n-Hexane may cause drowsiness.
(i) STOT-repeated exposure	n-Hexane may cause damage to the nervous system through inhalation
(j) aspiration hazard	n-Hexane may be fatal if swallowed and enters airways

The component n-Hexane has been extensively tested for REACH registration. 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.

n-Hexane: May cause peripheral nervous system disorder and/or damage. Blurred vision is associated with hexane polyneuropathy.

**Chronic Effects From Overexposure:**

No data available for product.

Hexane: Overexposure to n-hexane may cause progressive and potentially irreversible damage to the peripheral nervous system, particularly in the arms and legs. The neurotoxic effects of n-hexane vapour can be enhanced in rats by both methyl ethyl ketone (MEK) and lead acetate. The available information does not suggest that n-hexane is mutagenic. Negative results were obtained in most tests using live animals and relevant routes of exposure. n-Hexane has caused severe testicular damage in male rats at concentrations which have produced significant other toxicity.

**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 two components

The mixture is predicted to be Toxic to aquatic organisms based on hexane

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-Hexane:

Fish 96h LC<sub>50</sub> 8.2 mg/l

Daphnia 48h EC<sub>50</sub> 4.5 mg/l

Daphnia reproduction toxicity, NOEC for reproduction 5 mg/l

Algae 96h IC<sub>50</sub> 3.1 mg/l

**12.2 Persistence and degradability**

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

Hexane: Hexane readily volatilizes, biodegrades in soil, water and wastewater treatment plants, adsorbs to organic matter in aquatic systems, has low mobility in soil.

**12.3 Bioaccumulative potential**

n-Hexane : Log BCF = 2.24 to 2.89

**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	<b>UN Number</b>	UN3394
14.2	<b>UN proper shipping name (IMDG, ICAO, ADR, DOT)</b>	Organometallic substance, liquid, pyrophoric, water-reactive (n-butyllithium, hydrocarbon solution)
14.3	<b>Transport hazard class(es) (IMDG, ICAO, ADR, DOT)</b>	4.2, Spontaneously combustible, (4.3, Dangerous When Wet)
14.4	<b>Packing group (IMDG, ICAO, ADR, DOT)</b>	I
14.5	<b>Environmental hazards</b>	Marine pollutant due to presence of hexane
14.6	<b>Special precautions for user</b>	None
14.7	<b>Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code</b>	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)**

n-Butyllithium	not listed
n-hexane	2

#### 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 contains hexane which is a substance subject to the reporting requirements of Section 313 of the Emergency Planning and Community Right-To-Know Act of 1986.

This information must be included in all SDS's that are copied and distributed for this material.

Not listed

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

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

n-Hexane and hexanes are listed. The reportable quantity is 5000 pounds.

##### **TSCA Sec 12b Export Notification:**

This product is not subject to TSCA 12 (b) Export Notification Requirements.

##### **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 butyllithium as it is registered for use as a strictly controlled intermediate.

A chemical safety report has been prepared for hexane.

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## 16. Other Information

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#### **European Union:**

#### **R Phrases:**



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
Harmful: danger of serious damage to health by prolonged exposure through inhalation	R48/20
Possible risk of impaired fertility	R62
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

**Specific uses identified for Exposure Scenarios**

ES1	Receipt and use of butyllithium in hexane as chemical intermediate
ES2	Recovery of hexane

**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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