



SAFETY DATA SHEET

N-BUTYLLITHIUM IN HEPTANE

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

- 1.1 **Product Identifier:** n-Butyllithium in Heptane
1.1.1 **Substances** Not applicable
1.1.2 **Mixture name:** n-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
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
Fax: +44.151.482.7361

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
Web: 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, R65, 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 Phrases:

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
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]

Chemical Name	CAS #	EC No	EC Index No	REACH Reg No	Wt.%	Classification, Hazard Statement Codes
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
heptanes ¹	64742-49-0	927-510-4 (Provisional)	None	01-2119475515-33	69-90	Flam. Liq. 2 H225 Skin Irrit. 2 H315 Asp. Tox. 1 H304 STOT SE 3 H336 Aquatic Chronic 2 H411
Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich ²	None	925-292-5	None	01-2119474209-33-0016	0.1-3	Flam. Liq. 2 H225 Skin Irrit. 2 H315 Asp. Tox. 1 H304 Repr. 2 H361f STOT SE 3 H336 STOT RE 2 H373 Aquatic chronic 2 H411

¹ Contains n-heptane CAS# 142-82-5, and methylcyclohexane CAS# 108-87-2

² Contains n-hexane, CAS# 110-54-3

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
n-Butyllithium	109-72-8	203-698-7	10 - 31	F C	R14/15, R17; R34;
heptanes ¹	64742-49-0	927-510-4 (Provisional)	69-90	F; Xn; Xi; N;	R11 R65 R38 R67 R51/53
Hydrocarbons, C6, n-alkanes, iso-alkanes, cyclics, n-hexane rich ²	None	925-292-5	0.1-3	F; Xi; Xn; Repr.Cat.3; N;	R11 R38 R65, R67, R48/20 R62 R51/53

¹ Contains n-heptane CAS# 142-82-5, and methylcyclohexane CAS# 108-87-2

² 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.

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. n-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)

6. Accidental Release Measures

- 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.

7. Handling and Storage

- 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

8. Exposure Controls / Personal Protection

8.1 Control parameters

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

DNEL

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

Long-term exposure, systemic, inhalation 2085 mg/m³
 Long-term exposure, systemic, dermal 300 mg/kg/day

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

Long-term exposure, systemic, inhalation 93 mg/m³
 Long-term exposure, systemic, dermal 13 mg/kg/day

PNEC

Heptanes

Not determined by registrant.
 Estimated 0.01 using factor of 100

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

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	
n-hexane	20 ppm		20 ppm	60 ppm	50 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
 Quick-drench eyewash and safety shower.

Work Hygienic

Practices:

9. Physical and Chemical Properties

9.1 Information on basic physical and chemical properties

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

9.2 Other information

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

10. Stability and Reactivity

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

11. Toxicological Information

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	n-Butyllithium: Corrosive Heptanes: Oral LD ₅₀ >5840 mg/kg Inhalation LC ₅₀ >23300 mg/m ³ (rat, 4 hr)
(b) skin corrosion/irritation	Classified as corrosive on the basis of n-butyllithium.
(c) serious eye damage/irritation	Classified as corrosive on the basis of n-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	Heptanes and hexanes may cause drowsiness.
(i) STOT-repeated exposure	Hexanes may cause damage to the nervous system through inhalation
(j) aspiration hazard	Heptanes and hexanes may be fatal if swallowed and enters airways

The solvents have 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.

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

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.

12. Ecological Information

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 hexane and heptane.

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

Fish 96h LC₅₀ 109 mg/L

Daphnia 48h EC₅₀ 29 mg/L

Algae 96h IC₅₀ 3.4 mg/L

n-Hexane:

Fish 96h LC₅₀ 8.2 mg/L

Daphnia 48h EC₅₀ 4.5 mg/L

Algae 96h IC₅₀ 3.1 mg/L

n-Heptane:

Fish 96h LC₅₀ : not toxic within limits of water solubility

Daphnia 48h EC₅₀ : not toxic within limits of water solubility

Algae 96h IC₅₀ : not toxic within limits of water solubility

12.2 Persistence and degradability

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

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. BOD5 = 55% of ThOD. Heptane is not expected to bioaccumulate.

n-Hexane: Hexane readily volatilizes, biodegrades in soil, water and wastewater treatment plants, adsorbs to organic matter in aquatic systems, has low mobility in soil. Log BCF = 2.24 to 2.89.

12.3 **Bioaccumulative potential**

n-Hexane : Log BCF = 2.24 to 2.89
Heptane is not expected to bioaccumulate

12.4 **Mobility in soil**

Not available.

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.

13. Disposal Considerations

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.

14. Transport Information

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

15. Regulatory Information

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
heptane	3
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):

TSCA Sec 12b Export Notification:

NFPA Rating:

n-Hexane and heptanes are listed. The reportable quantities are respectively 5000 lbs and 5000 lbs.

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

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

INTERNATIONAL INVENTORY STATUS:

<u>Inventory/Country</u>	<u>Product Status</u>
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 heptanes.

16. Other Information

European Union:

R Phrases:	
Reacts violently with water, liberating extremely flammable gases	R14/15
Spontaneously flammable in air	R17
Highly flammable.	R11
Irritating to skin.	R38
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 heptane as chemical intermediate
ES2	Recovery of heptane including use in fuels

REVISION SUMMARY: Revision # 2. Sections 2, 3, 11, 12, 15 and 16 changed. Added hexane impurity.

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

type 4

Copyright 2017. FMC Corporation. All Rights Reserved. FMC and the FMC logo are trademarks of FMC Corporation.

References

Supplier SDS for Heptane

Disseminated Dossiers for Heptane
Source: European Chemicals Agency, <http://echa.europa.eu/>