



SAFETY DATA SHEET

N-BUTYLLITHIUM IN TOLUENE

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

- 1.1 **Product Identifier:** n-Butyllithium in Toluene
1.1.1 **Substances** Not applicable
1.1.2 **Mixture name:** n-Butyllithium in Toluene
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

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, R63;

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 the unborn child. H361d
 May cause damage to organs through prolonged or repeated exposure. H373

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 Statements(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

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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n-Butyllithium	109-72-8	203-698-7	None	01-2119494906-21-0001	10 - 31	Pyr. Liq. 1 Water-react. 1 Skin Corr. 1B	H250 H260 H314
Toluene	108-88-3	203-625-9	601-021-00-3	01-2119471310-51-****	60-92	Flam. liq. 2 Skin Irrit. 2 Asp. Tox.1 Repr. 2 STOT SE 3 STOT RE 2	H225 H315 H304 H361d H336 H373

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;
Toluene	108-88-3	203-625-9	60-92	F; Xi; Xn; Repr.Cat.3;	R11 R38 R48/20-65 R63 R67

(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** Estimated 4 °C (Closed Cup) based on toluene.
- Flammable limits in air** Not applicable for formulation. For toluene: Upper: 7.1 wt%
Lower: 1.1 wt%
- Auto ignition temperature** Not applicable for formulation. n-Butyllithium in toluene 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

Toluene

Long-term exposure, systemic, inhalation	192 mg/m ³
Long-term exposure, systemic, dermal	384 mg/kg/day

PNEC

Toluene

Freshwater	0.68 mg/L
Marine	0.68 mg/L

EXPOSURE LIMITS

Chemical Name	EU		EH40 (UK WEL)		USA (ACGIH)		USA (OSHA)	
	TWA	STEL	TWA	STEL	TWA	STEL/Ceiling	PEL	STEL/Ceiling
toluene	50 ppm	100 ppm	50 ppm	100 ppm	20 ppm		200 ppm	300 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.

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>	110.6 °C (toluene)
<u>Flash point:</u>	Estimated 4 °C (Closed Cup) based on toluene.
<u>Evaporation rate(butyl acetate = 1):</u>	2.10 (toluene)
<u>Flammability:</u>	Pyrophoric and water reactive material in flammable liquid solvent
<u>Flammable limits:</u>	Not applicable for formulation. For toluene: Upper: 7.1 wt% Lower: 1.1 wt%
<u>Vapor pressure:</u>	2.93 kPa (22 mm Hg) at 20 °C (toluene)
<u>Vapor density (air = 1):</u>	3.1 (toluene)
<u>Specific gravity:</u>	0.7-0.8 g.ml @ 20 °C (68 °F)
<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 toluene is pyrophoric at room temperature and 50% humidity.
<u>Decomposition temperature:</u>	Not available
<u>Viscosity:</u>	Contains low viscosity hydrocarbons
<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 toluene is pyrophoric.
<u>Self-heating properties</u>	Does not meet classification criteria.
<u>Water reactive properties</u>	n-Butyllithium in toluene is a packing group I water reactive.
<u>Corrosive to metals</u>	Does not meet classification criteria.

Molecular weight: 64.06

10. Stability and Reactivity

10.1	<u>Reactivity</u>	Reactive with water and damp air
10.2	<u>Chemical stability</u>	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	Butyllithium: Corrosive Toluene: Acute Oral LD ₅₀ = 636 mg/kg (rat) Toluene: Acute Dermal LD ₅₀ = 14100 uL/kg (rabbit) Toluene: Acute inhalation LC ₅₀ = 49 gm/m ³ /4H (rat)
(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	Toluene suspected of damaging fertility or the unborn child.
(h) STOT-single exposure	Toluene may cause drowsiness.
(i) STOT-repeated exposure	Toluene may cause damage to organs through inhalation
(j) aspiration hazard	Toluene may be fatal if swallowed and enters airways

The component toluene 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.

Chronic Effects From Overexposure:

No data available for product.

Toluene: Possible reproductive hazard - may cause developmental toxicity, based on animal information. Toluene was not carcinogenic in mice and rats exposed by inhalation to up to 1200 ppm for 24 months. Prolonged skin exposure may result in dermatitis. Symptoms observed in laboratory animals following subchronic inhalation exposure to toluene has caused narcosis, tremors and anesthesia in laboratory animals.

Prolonged contact with toluene may cause defatting of the skin and skin irritation.

Carcinogenicity Listings

Eh40: Not listed.
IARC: Group 3 (Not Classifiable)
NTP: Not listed.
OSHA: Not considered a carcinogen under OSHA.
ACGIH: A4 - Not Classifiable as a Human Carcinogen

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 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

Toluene

Acute LC₅₀ (fish) = 5.5 mg/l

Acute LC₅₀ (daphnia) = 3.4 mg/l

EC₅₀ (algae) = 10 mg/l

Daphnia reproduction, NOEC 3.2 mg/l

12.2 Persistence and degradability

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

Toluene: Toluene biodegrades slowly and volatilizes rapidly from soil. It is not expected to bioconcentrate.

12.3 Bioaccumulative potential

Toluene is not expected to bioaccumulate.

12.4 Mobility in soil

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.

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 UN Number

UN3394

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

Organometallic substance, liquid, pyrophoric, water-reactive (n-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)

I

14.5 Environmental hazards

None

14.6 Special precautions for user

None

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

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
toluene	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 toluene which is 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): Toluene is listed. The reportable quantity is 1000 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:

<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 toluene.

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 harm to the unborn child.	R63
Vapours may cause drowsiness and dizziness.	R67
Highly flammable liquid and vapour.	H225
Catches fire spontaneously if exposed to air	H250
In contact with water releases flammable gases, which may ignite spontaneously.	H260
May be fatal if swallowed and enters airways	H304
Causes severe skin burns and eye damage.	H314
Causes skin irritation	H315
May cause drowsiness or dizziness.	H336
Suspected of damaging fertility or the unborn child	H361d
May cause damage to organs through prolonged or repeated exposure.	H373

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 # 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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References

Supplier SDS for Toluene

Disseminated Dossiers for Toluene

Source: European Chemicals Agency, <http://echa.europa.eu/>