

## SAFETY DATA SHEET

Revision Date 25-Dec-2021

Revision Number 4

### 1. Identification

**Product Name** Isobutyllithium, 1.7M solution in heptane

**Cat No. :** AC377590000; AC377591000; AC377598000

**Synonyms** No information available

**Recommended Use** Laboratory chemicals.

**Uses advised against** Food, drug, pesticide or biocidal product use.

#### Details of the supplier of the safety data sheet

##### Company

Fisher Scientific Company  
One Reagent Lane  
Fair Lawn, NJ 07410  
Tel: (201) 796-7100

Acros Organics  
One Reagent Lane  
Fair Lawn, NJ 07410

**Emergency Telephone Number** For information **US** call: 001-800-ACROS-01 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No.**US**:001-800-424-9300 / **Europe**:001-703-527-3887

### 2. Hazard(s) identification

#### Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Flammable liquids	Category 2
Substances/mixtures which, in contact with water, emit flammable gases	Category 1
Pyrophoric liquids	Category 1
Skin Corrosion/Irritation	Category 1 A
Serious Eye Damage/Eye Irritation	Category 1
Reproductive Toxicity	Category 2
Specific target organ toxicity (single exposure)	Category 3
Target Organs - Central nervous system (CNS).	
Specific target organ toxicity - (repeated exposure)	Category 2
Aspiration Toxicity	Category 1

#### Label Elements

**Signal Word**  
Danger

**Hazard Statements**

Highly flammable liquid and vapor  
In contact with water releases flammable gases which may ignite spontaneously  
Catches fire spontaneously if exposed to air  
May be fatal if swallowed and enters airways  
Causes severe skin burns and eye damage  
May cause drowsiness or dizziness  
Suspected of damaging fertility or the unborn child  
May cause damage to organs through prolonged or repeated exposure

**Precautionary Statements****Prevention**

Obtain special instructions before use  
Do not handle until all safety precautions have been read and understood  
Wear protective gloves/protective clothing/eye protection/face protection  
Do not breathe dust/fume/gas/mist/vapors/spray  
Wash face, hands and any exposed skin thoroughly after handling  
Use only outdoors or in a well-ventilated area  
Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
Keep container tightly closed  
Ground/bond container and receiving equipment  
Use explosion-proof electrical/ventilating/lighting equipment  
Use only non-sparking tools  
Take precautionary measures against static discharge  
Do not allow contact with air  
Keep away from any possible contact with water, because of violent reaction and possible flash fire  
Handle under inert gas. Protect from moisture  
Keep cool

**Response**

Get medical attention/advice if you feel unwell  
IF exposed or concerned: Get medical attention/advice

**Inhalation**

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

**Skin**

IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower  
Wash contaminated clothing before reuse  
Immediately call a POISON CENTER or doctor/physician

**Eyes**

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
Immediately call a POISON CENTER or doctor/physician

**Ingestion**

Do NOT induce vomiting  
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician  
IF SWALLOWED: Rinse mouth. DO NOT induce vomiting

**Fire**

In case of fire: Use CO<sub>2</sub>, dry chemical, or foam for extinction

**Storage**

Store locked up  
Store in a well-ventilated place. Keep container tightly closed  
Store contents under inert gas  
Store in a dry place. Store in a closed container

Store away from other materials

**Disposal**

Dispose of contents/container to an approved waste disposal plant

**Hazards not otherwise classified (HNOC)**

Toxic to aquatic life with long lasting effects

Reacts violently with water

### 3. Composition/Information on Ingredients

Component	CAS No	Weight %
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	64742-49-0	84
Isobutyllithium	920-36-5	16

### 4. First-aid measures

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
<b>Inhalation</b>	Remove from exposure, lie down. Remove to fresh air. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required. If not breathing, give artificial respiration. Risk of serious damage to the lungs (by aspiration).
<b>Ingestion</b>	Do NOT induce vomiting. Call a physician or poison control center immediately. If vomiting occurs naturally, have victim lean forward.
<b>Most important symptoms and effects</b>	Difficulty in breathing. Causes burns by all exposure routes. Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation
<b>Notes to Physician</b>	Treat symptomatically

### 5. Fire-fighting measures

<b>Suitable Extinguishing Media</b>	Dry chemical, soda ash, lime or sand. approved class D extinguishers. Water mist may be used to cool closed containers.
<b>Unsuitable Extinguishing Media</b>	DO NOT USE WATER
<b>Flash Point</b>	No information available
<b>Method -</b>	No information available
<b>Autoignition Temperature</b>	204 °C / 399.2 °F
<b>Explosion Limits</b>	
<b>Upper</b>	6.7%
<b>Lower</b>	1.05%
<b>Sensitivity to Mechanical Impact</b>	No information available
<b>Sensitivity to Static Discharge</b>	No information available

**Specific Hazards Arising from the Chemical**

Flammable. Contact with water liberates toxic gas. Water reactive. Pyrophoric: Spontaneously flammable in air. Produce flammable gases on contact with water. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

**Hazardous Combustion Products**

Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Isobutane.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**NFPA**

**Health**  
3

**Flammability**  
4

**Instability**  
2

**Physical hazards**  
W

**6. Accidental release measures****Personal Precautions**

Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

Do not flush into surface water or sanitary sewer system.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Do not expose spill to water.

**7. Handling and storage****Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not breathe mist/vapors/spray. Do not get in eyes, on skin, or on clothing. Handle product only in closed system or provide appropriate exhaust ventilation. Use spark-proof tools and explosion-proof equipment. Use only non-sparking tools. Do not allow contact with water. Do not allow contact with water because of violent reaction. Keep away from open flames, hot surfaces and sources of ignition. To avoid ignition of vapors by static electricity discharge, all metal parts of the equipment must be grounded. Take precautionary measures against static discharges.

**Storage.**

Keep container tightly closed. Keep away from heat, sparks and flame. Protect from direct sunlight. Store in freezer. Keep from any possible contact with water. Corrosives area. Flammables area. Keep under nitrogen. Keep containers tightly closed in a dry, cool and well-ventilated place. Incompatible Materials. Acids. Water. Strong oxidizing agents. Alcohols. Carbon dioxide (CO<sub>2</sub>).

**8. Exposure controls / personal protection****Exposure Guidelines****Engineering Measures**

Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

**Personal Protective Equipment****Eye/face Protection**

Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

**Skin and body protection**

Wear appropriate protective gloves and clothing to prevent skin exposure.

**Respiratory Protection**

Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard

EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

**Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

## 9. Physical and chemical properties

<b>Physical State</b>	Liquid
<b>Appearance</b>	Light yellow
<b>Odor</b>	Petroleum distillates
<b>Odor Threshold</b>	No information available
<b>pH</b>	Not applicable
<b>Melting Point/Range</b>	No data available
<b>Boiling Point/Range</b>	No information available
<b>Flash Point</b>	No information available
<b>Evaporation Rate</b>	No information available
<b>Flammability (solid,gas)</b>	Not applicable
<b>Flammability or explosive limits</b>	
Upper	6.7%
Lower	1.05%
<b>Vapor Pressure</b>	No information available
<b>Vapor Density</b>	No information available
<b>Specific Gravity</b>	0.700
<b>Solubility</b>	Reacts violently with water
<b>Partition coefficient; n-octanol/water</b>	No data available
<b>Autoignition Temperature</b>	204 °C / 399.2 °F
<b>Decomposition Temperature</b>	No information available
<b>Viscosity</b>	No information available
<b>Molecular Formula</b>	C <sub>4</sub> H <sub>9</sub> Li
<b>Molecular Weight</b>	64.06

## 10. Stability and reactivity

<b>Reactive Hazard</b>	Yes
<b>Stability</b>	Reacts violently with water. Moisture sensitive. Air sensitive. Light sensitive. Pyrophoric: Spontaneously flammable in air.
<b>Conditions to Avoid</b>	Keep away from open flames, hot surfaces and sources of ignition. Exposure to air. Exposure to light. Incompatible products. Exposure to moist air or water.
<b>Incompatible Materials</b>	Acids, Water, Strong oxidizing agents, Alcohols, Carbon dioxide (CO <sub>2</sub> )
<b>Hazardous Decomposition Products</b>	Carbon monoxide (CO), Carbon dioxide (CO <sub>2</sub> ), Isobutane
<b>Hazardous Polymerization</b>	No information available.
<b>Hazardous Reactions</b>	None under normal processing.

## 11. Toxicological information

**Acute Toxicity****Product Information**

**Oral LD50** Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.

**Dermal LD50** Based on ATE data, the classification criteria are not met. ATE > 2000 mg/kg.

**Vapor LC50** Based on ATE data, the classification criteria are not met. ATE > 20 mg/l.

**Component Information**

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Hydrocarbons, C <sub>6</sub> , n-alkanes, isoalkanes, cyclics, n-hexane rich	LD50 > 5000 mg/kg ( Rat )	LD50 > 3160 mg/kg ( Rabbit )	LC50 = 73680 ppm ( Rat ) 4 h

**Toxicologically Synergistic Products** No information available

**Delayed and immediate effects as well as chronic effects from short and long-term exposure**

**Irritation** No information available

**Sensitization** No information available

**Carcinogenicity** The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	64742-49-0	Not listed	Not listed	Not listed	Not listed	Not listed
Isobutyllithium	920-36-5	Not listed	Not listed	Not listed	Not listed	Not listed

**Mutagenic Effects** No information available

**Reproductive Effects** No information available.

**Developmental Effects** No information available.

**Teratogenicity** No information available.

**STOT - single exposure** Central nervous system (CNS)

**STOT - repeated exposure** None known

**Aspiration hazard** No information available

**Symptoms / effects, both acute and delayed** Inhalation of high vapor concentrations may cause symptoms like headache, dizziness, tiredness, nausea and vomiting: Product is a corrosive material. Use of gastric lavage or emesis is contraindicated. Possible perforation of stomach or esophagus should be investigated: Ingestion causes severe swelling, severe damage to the delicate tissue and danger of perforation

**Endocrine Disruptor Information** No information available

**Other Adverse Effects** The toxicological properties have not been fully investigated.

## 12. Ecological information

### Ecotoxicity

Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment. The product contains following substances which are hazardous for the environment.

Component	Freshwater Algae	Freshwater Fish	Microtox	Water Flea
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	Not listed	LC50: = 8.41 mg/L, 96h semi-static, closed (Oncorhynchus mykiss)	Not listed	Not listed

**Persistence and Degradability** Soluble in water Persistence is unlikely based on information available.

**Bioaccumulation/ Accumulation** No information available.

**Mobility** . Will likely be mobile in the environment due to its water solubility.

## 13. Disposal considerations

**Waste Disposal Methods** Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## 14. Transport information

**DOT**

**UN-No** UN3394  
**Proper Shipping Name** ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE  
**Technical Name** (ISOBUTYLLITHIUM, HEPTANE)  
**Hazard Class** 4.2  
**Subsidiary Hazard Class** 4.3, 3, 8  
**Packing Group** I

**TDG**

**UN-No** UN3394  
**Proper Shipping Name** ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE  
**Hazard Class** 4.2  
**Subsidiary Hazard Class** 4.3, 3, 8  
**Packing Group** I

**IATA**

**UN-No** UN3394  
**Proper Shipping Name** ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE,  
**Hazard Class** 4.2  
**Subsidiary Hazard Class** 4.3

**IMDG/IMO**

**UN-No** UN3394  
**Proper Shipping Name** ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE  
**Hazard Class** 4.2  
**Subsidiary Hazard Class** 4.3  
**Packing Group** I

## 15. Regulatory information

**United States of America Inventory**

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	64742-49-0	X	ACTIVE	-
Isobutyllithium	920-36-5	-	-	-

**Legend:**

**TSCA** US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

- - Not Listed

**TSCA 12(b)** - Notices of Export Not applicable

**International Inventories**

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	64742-49-0	X	-	265-151-9	X	-		X	X	KE-25623
Isobutyllithium	920-36-5	-	-	-	-	X	X	-	-	-

**KECL** - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

**U.S. Federal Regulations**

**SARA 313** Not applicable

**SARA 311/312 Hazard Categories** See section 2 for more information

**CWA (Clean Water Act)** Not applicable

**Clean Air Act** Not applicable

**OSHA - Occupational Safety and Health Administration** Not applicable

**CERCLA** Not applicable

**California Proposition 65** This product does not contain any Proposition 65 chemicals.

**U.S. State Right-to-Know Regulations**

**U.S. Department of Transportation**

Reportable Quantity (RQ): N  
DOT Marine Pollutant N  
DOT Severe Marine Pollutant N

**U.S. Department of Homeland Security** This product does not contain any DHS chemicals.

**Other International Regulations**

**Mexico - Grade** No information available

**Authorisation/Restrictions according to EU REACH**

Component	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	-	Use restricted. See item 28. (see link for restriction details) Use restricted. See item 29. (see link for restriction details) Use restricted. See item 75. (see link for restriction details)	-
Isobutyllithium	-	Use restricted. See item 75. (see link for restriction details)	-

<https://echa.europa.eu/substances-restricted-under-reach>

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	64742-49-0	Listed	Not applicable	Not applicable	Not applicable
Isobutyllithium	920-36-5	Not applicable	Not applicable	Not applicable	Not applicable

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Hydrocarbons, C6, n-alkanes, isoalkanes, cyclics, n-hexane rich	64742-49-0	Not applicable	Not applicable	Not applicable	Not applicable



Isobutyllithium	920-36-5	Not applicable	Not applicable	Not applicable	Not applicable
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## 16. Other information

**Prepared By**

Regulatory Affairs  
Thermo Fisher Scientific  
Email: EMSDS.RA@thermofisher.com

**Revision Date**

25-Dec-2021

**Print Date**

25-Dec-2021

**Revision Summary**

This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of SDS**