

## SAFETY DATA SHEET

Version 6.8  
Revision Date 11/14/2023  
Print Date 01/13/2024**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**Product name : *tert*-Butyllithium solutionProduct Number : 186198  
Brand : Aldrich**1.2 Relevant identified uses of the substance or mixture and uses advised against**

Identified uses : Laboratory chemicals, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATESTelephone : +1 314 771-5765  
Fax : +1 800 325-5052**1.4 Emergency telephone**Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-  
527-3887 CHEMTREC (International) 24  
Hours/day; 7 Days/week**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**Flammable liquids (Category 2), H225  
Pyrophoric liquids (Category 1), H250  
Chemicals which, in contact with water, emit flammable gases (Category 1), H260  
Skin corrosion (Category 1B), H314  
Serious eye damage (Category 1), H318  
Specific target organ toxicity - single exposure (Category 3), Central nervous system, H336  
Aspiration hazard (Category 1), H304  
Short-term (acute) aquatic hazard (Category 2), H401  
Long-term (chronic) aquatic hazard (Category 2), H411

For the full text of the H-Statements mentioned in this Section, see Section 16.

## 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard statement(s)

H225 Highly flammable liquid and vapor.  
H250 Catches fire spontaneously if exposed to air.  
H260 In contact with water releases flammable gases which may ignite spontaneously.  
H304 May be fatal if swallowed and enters airways.  
H314 Causes severe skin burns and eye damage.  
H336 May cause drowsiness or dizziness.  
H411 Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

P210 Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.  
P222 Do not allow contact with air.  
P223 Do not allow contact with water.  
P231 + P232 Handle under inert gas. Protect from moisture.  
P233 Keep container tightly closed.  
P240 Ground/bond container and receiving equipment.  
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.  
P242 Use only non-sparking tools.  
P243 Take precautionary measures against static discharge.  
P261 Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.  
P264 Wash skin thoroughly after handling.  
P271 Use only outdoors or in a well-ventilated area.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER/ doctor.  
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.  
P302 + P334 IF ON SKIN: Immerse in cool water/ wrap in wet bandages.  
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.  
P304 + P340 + P310 IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.  
P305 + P351 + P338 + P310 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/ doctor.  
P335 + P334 Brush off loose particles from skin. Immerse in cool water/ wrap in wet bandages.  
P363 Wash contaminated clothing before reuse.  
P370 + P378 In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.  
P391 Collect spillage.  
P402 + P404 Store in a dry place. Store in a closed container.  
P403 + P233 Store in a well-ventilated place. Keep container tightly closed.  
P403 + P235 Store in a well-ventilated place. Keep cool.

P405	Store locked up.
P422	Store contents under inert gas.
P501	Dispose of contents/ container to an approved waste disposal plant.

### 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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## SECTION 3: Composition/information on ingredients

### 3.2 Mixtures

Synonyms : Lithium-2-methyl-2-propanide  
t-BuLi

Formula : C<sub>4</sub>H<sub>9</sub>Li  
Molecular weight : 64.06 g/mol

Component	Classification	Concentration
<b>pentane</b>		
CAS-No. 109-66-0 EC-No. 203-692-4 Index-No. 601-006-00-1 Registration number 01-2119459286-30-XXXX	Flam. Liq. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 2; Aquatic Chronic 2; H225, H336, H304, H401, H411 Concentration limits: 20 %: STOT SE 3, H336;	>= 70 - < 90 %
<b>lithium-tert-butylate</b>		
CAS-No. 594-19-4 EC-No. 209-831-5	Pyr. Liq. 1; Water-react 1; Skin Corr. 1B; Eye Dam. 1; H250, H260, H314, H318	>= 10 - < 20 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Take off contaminated clothing and shoes immediately. Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician. Continue rinsing eyes during transport to hospital.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

**4.3 Indication of any immediate medical attention and special treatment needed**

No data available

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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Dry powder Dry powder Carbon dioxide (CO<sub>2</sub>)

**Unsuitable extinguishing media**

Water Carbon dioxide (CO<sub>2</sub>) Water

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides  
Lithium oxides  
Combustible.

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

No data available

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Do not flush with water.

## 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

#### Advice on protection against fire and explosion

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

#### Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

For precautions see section 2.2.

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

#### Storage conditions

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Never allow product to get in contact with water during storage.

#### Storage stability

Recommended storage temperature

2 - 8 °C

Air and moisture sensitive. Handle and store under inert gas. Sensitive to carbon dioxide

#### Storage class

Storage class (TRGS 510): 4.2: Pyrophoric and self-heating hazardous materials

### 7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
pentane	109-66-0	C	610 ppm 1,800 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	120 ppm 350 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	1,000 ppm 2,950 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	600 ppm 1,800 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		TWA	1,000 ppm	USA. ACGIH Threshold Limit Values (TLV)

## 8.2 Exposure controls

### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### Personal protective equipment

#### Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### Body Protection

Choose body protection according to the amount and concentration of the dangerous substance at the work place., Flame retardant antistatic protective clothing., Antistatic boots

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: light yellow
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	No data available
f) Initial boiling point and boiling range	No data available
g) Flash point	-49 °C (-56 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.652 g/mL at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	No data available

- o) Partition coefficient: No data available  
n-octanol/water
- p) Autoignition No data available  
temperature
- q) Decomposition No data available  
temperature
- r) Viscosity No data available
- s) Explosive properties Not classified as explosive.
- t) Oxidizing properties none

## 9.2 Other safety information

No data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.  
Reacts violently with water.

### 10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight. Exposure to moisture.

### 10.5 Incompatible materials

acids, Water, Alcohols, Carbon dioxide (CO<sub>2</sub>), Humid air, Halogenated hydrocarbon, Amines

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Mixture

#### Acute toxicity

Oral: No data available

Oral: No data available

Acute toxicity estimate Inhalation - 4 h - 30.12 mg/l - vapor(Calculation method)

Dermal: No data available



No data available

**Skin corrosion/irritation**

Remarks: No data available

**Serious eye damage/eye irritation**

Remarks: No data available

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

No data available

**Carcinogenicity**

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

**Reproductive toxicity**

No data available

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

burning sensation, Cough, wheezing, laryngitis, Shortness of breath, spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Liver - Irregularities - Based on Human Evidence

## Components

### pentane

#### Acute toxicity

LD50 Oral - Rat - male and female - > 2,000 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 25.3 mg/l - vapor

(OECD Test Guideline 403)

Remarks: (in analogy to similar products)

The value is given in analogy to the following substances: cyclopentane

Dermal: No data available

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

#### Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Method: Mutagenicity (micronucleus test)

Species: Rat - male and female - Bone marrow

Result: negative

#### Carcinogenicity

No data available

#### Reproductive toxicity

No data available

#### Specific target organ toxicity - single exposure

May cause drowsiness or dizziness. - Central nervous system

#### Specific target organ toxicity - repeated exposure

No data available

#### Aspiration hazard

May be fatal if swallowed and enters airways. Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

## **lithium-tert-butylate**

### **Acute toxicity**

Oral: No data available  
Inhalation: No data available  
Dermal: No data available  
No data available

### **Skin corrosion/irritation**

Remarks: No data available

### **Serious eye damage/eye irritation**

No data available

### **Respiratory or skin sensitization**

No data available

### **Germ cell mutagenicity**

No data available

### **Carcinogenicity**

No data available

### **Reproductive toxicity**

No data available  
No data available

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

#### **Mixture**

No data available

### **12.2 Persistence and degradability**

No data available

### **12.3 Bioaccumulative potential**

No data available

### **12.4 Mobility in soil**

No data available

### **12.5 Results of PBT and vPvB assessment**

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

## 12.6 Endocrine disrupting properties

No data available

## 12.7 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Toxic to aquatic life.

### Components

#### pentane

Toxicity to fish	static test LC50 - Oncorhynchus mykiss (rainbow trout) - 4.26 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 2.7 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	static test ErC50 - Selenastrum capricornutum (green algae) - 10.7 mg/l - 72 h (OECD Test Guideline 201)  static test NOEC - Selenastrum capricornutum (green algae) - 7.51 mg/l - 72 h (OECD Test Guideline 201)

#### lithium-tert-butylate

No data available

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

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UN number: 3394 Class: 4.2 (4.3) Packing group: I  
Proper shipping name: Organometallic substance, liquid, pyrophoric, water-reactive  
(lithium-tert-butylate)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

**IMDG**

UN number: 3394 Class: 4.2 (4.3) Packing group: I EMS-No: F-G, S-M  
Proper shipping name: ORGANOMETALLIC SUBSTANCE, LIQUID, PYROPHORIC, WATER-REACTIVE (lithium-tert-butylate)  
Marine pollutant : yes

**IATA**

UN number: 3394 Class: 4.2 (4.3)  
Proper shipping name: Organometallic substance, liquid, pyrophoric, water-reactive  
(lithium-tert-butylate)  
IATA Passenger: Not permitted for transport  
IATA Cargo: Not permitted for transport

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**SECTION 15: Regulatory information**

**SARA 302 Components**

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Fire Hazard, Reactivity Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

	CAS-No.	Revision Date
pentane	109-66-0	1993-02-16

**Pennsylvania Right To Know Components**

	CAS-No.	Revision Date
pentane	109-66-0	1993-02-16

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## SECTION 16: Other information

### Further information

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