SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: sec-Butyllithium solution
Product Number: 195596
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 STATES

Telephone: +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 1), H400
- Long-term (chronic) aquatic hazard (Category 1), H410

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

2.2 GHS Label elements, including precautionary statements

Aldrich - 195596
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada.
2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures
Synonyms: Lithium-2-butanide s-BuLi

Formula: C₄H₉Li
Molecular weight: 64.06 g/mol

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclohexane</td>
<td>Flam. Liq. 2; Skin Irrit. 2; STOT SE 3; Asp. Tox. 1; Aquatic Acute 1; Aquatic Chronic 1; H225, H315, H336, H304, H400, H410 Concentration limits: 20 %: STOT SE 3, H336; M-Factor - Aquatic Acute: 1</td>
<td>&gt;= 90 - &lt;= 100 %</td>
</tr>
<tr>
<td>sec-Butyllithium</td>
<td>Pyr. Liq. 1; Water-react 1; Skin Corr. 1B; Eye Dam. 1; H250, H260, H314, H318</td>
<td>&gt;= 10 - &lt; 20 %</td>
</tr>
</tbody>
</table>

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

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice
First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled
After inhalation: fresh air. Call in physician.

In case of skin contact
In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact
After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.
**If swallowed**
After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Pulmonary failure possible after aspiration of vomit. Call a physician immediately. Do not attempt to neutralise.

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*
Carbon dioxide (CO2) Dry powder

*Unsuitable extinguishing media*
Water Foam

5.2 **Special hazards arising from the substance or mixture**
Carbon oxides
Combustible.
Pay attention to flashback.
Vapors are heavier than air and may spread along floors.
May not get in touch with: Water
Development of hazardous combustion gases or vapours possible in the event of fire.
Forms explosive mixtures with air at ambient temperatures.

5.3 **Advice for firefighters**
Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 **Further information**
Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

**SECTION 6: Accidental release measures**

6.1 **Personal precautions, protective equipment and emergency procedures**
Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert.
For personal protection see section 8.

6.2 **Environmental precautions**
Do not let product enter drains. Risk of explosion.

6.3 **Methods and materials for containment and cleaning up**
Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.
6.4 Reference to other sections
For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling
Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols. Keep workplace dry. Do not allow product to come into contact with water.

Advice on protection against fire and explosion
Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions
Tightly closed. Keep away from heat and sources of ignition. Never allow product to get in contact with water during storage.

Storage stability
Recommended storage temperature 2 - 8 °C  
Air sensitive. Handle and store under inert gas.

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters
### Component

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclohexane</td>
<td>110-82-7</td>
<td>TWA</td>
<td>100 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>300 ppm 1,050 mg/m³</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td></td>
<td></td>
<td>TWA</td>
<td>300 ppm 1,050 mg/m³</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td></td>
<td></td>
<td>PEL</td>
<td>300 ppm 1,050 mg/m³</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

### Biological occupational exposure limits

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Parameters</th>
<th>Value</th>
<th>Biological specimen</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclohexane</td>
<td>110-82-7</td>
<td>1,2-Cyclohexanediol</td>
<td>50mg/g creatinine</td>
<td>Urine</td>
<td>ACGIH - Biological Exposure Indices (BEI)</td>
</tr>
</tbody>
</table>

### 8.2 Exposure controls

#### Appropriate engineering controls
Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

#### Personal protective equipment

**Eye/face protection**
Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles.

**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: 0.11 mm
  - Break through time: 480 min
  - Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

- **Splash contact**
  - Material: Nitrile rubber
  - Minimum layer thickness: 0.11 mm
  - Break through time: 480 min
  - Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

- Remarks: End of shift at end of workweek

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada
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**
Flame retardant antistatic protective clothing.

**Respiratory protection**
required when vapours/aerosols are generated.
Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**
Do not let product enter drains. Risk of explosion.

### SECTION 9: Physical and chemical properties

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

- **Appearance**: Form: liquid
- **Odor**: No data available
- **Odor Threshold**: No data available
- **pH**: No data available
- **Melting point/freezing point**: No data available
- **Initial boiling point and boiling range**: No data available
- **Flash point**: -17 °C (1 °F) - closed cup
- **Evaporation rate**: No data available
- **Flammability (solid, gas)**: No data available
- **Upper/lower flammability or explosive limits**: No data available
- **Vapor pressure**: No data available
- **Vapor density**: No data available
- **Density**: 0.769 g/cm³
- **Relative density**: No data available
- **Water solubility**: No data available
- **Partition coefficient: n-octanol/water**: No data available
<p>| | |</p>
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<thead>
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<tbody>
<tr>
<td>p)</td>
<td>Autoignition temperature</td>
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<tr>
<td>q)</td>
<td>Decomposition temperature</td>
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<tr>
<td>r)</td>
<td>Viscosity</td>
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<tr>
<td>s)</td>
<td>Explosive properties</td>
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<tr>
<td>t)</td>
<td>Oxidizing properties</td>
</tr>
</tbody>
</table>

9.2 Other safety information
No data available

SECTION 10: Stability and reactivity

10.1 Reactivity
Vapors may form explosive mixture with air.

10.2 Chemical stability
Sensitive to air.

10.3 Possibility of hazardous reactions
No data available

10.4 Conditions to avoid
Exposure to air.
Warming.
Moisture.

10.5 Incompatible materials
Water, Strong oxidizing agents, Alcohols, acids

10.6 Hazardous decomposition products
In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

   Mixture

   **Acute toxicity**
   Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

   Inhalation: No data available
   Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract
   Dermal: No data available
Acute toxicity estimate Dermal - 2,778 mg/kg (Calculation method)

**Skin corrosion/irritation**
Remarks: Mixture causes burns.

**Serious eye damage/eye irritation**
Remarks: Mixture causes serious eye damage.
Risk of blindness!

**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

**Specific target organ toxicity - single exposure**
Mixture may cause drowsiness or dizziness.

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

### 11.2 Additional Information

Central nervous system depression, Drowsiness, Irritability, Dizziness, Damage to the lungs., Gastrointestinal disturbance, Lung irritation, chest pain, pulmonary edema, Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis
Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

**Components**

**Cyclohexane**

**Acute toxicity**
LD50 Oral - Rat - male and female - > 5,000 mg/kg
(OECID Test Guideline 401)
Symptoms: gastric pain, Stomach/intestinal disorders
LC50 Inhalation - Rat - male and female - 4 h - 19.07 mg/l - vapor
(OECD Test Guideline 403)
Symptoms: Possible damages:, Irritation symptoms in the respiratory tract., Inhalation may lead to the formation of oedemas in the respiratory tract.
LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

**Skin corrosion/irritation**
Remarks: Causes skin irritation.
Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

**Serious eye damage/eye irritation**
Remarks: No data available

**Respiratory or skin sensitization**
Buehler Test - Guinea pig
Result: negative

**Germ cell mutagenicity**
Test Type: Ames test
Test system: Salmonella typhimurium
Result: negative
Test Type: In vitro mammalian cell gene mutation test
Test system: Mouse lymphoma test
Result: negative
Method: OECD Test Guideline 475
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.
Acute oral toxicity - gastric pain, Stomach/intestinal disorders
Acute inhalation toxicity - Possible damages:, Irritation symptoms in the respiratory tract., Inhalation may lead to the formation of oedemas in the respiratory tract.

**Specific target organ toxicity - repeated exposure**
**Aspiration hazard**
May be fatal if swallowed and enters airways. Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

**sec-Butyllithium**

**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**
Remarks: 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

**Specific target organ toxicity - single exposure**
No data available

**Specific target organ toxicity - repeated exposure**
No data available

**Aspiration hazard**
No data available

---

**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**
No data available

**Components**

**Cyclohexane**
Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) - 4.53 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates: static test EC50 - Daphnia magna (Water flea) - 0.9 mg/l - 48h (OECD Test Guideline 202)

Toxicity to algae: ErC50 - Pseudokirchneriella subcapitata (green algae) - >4.425 mg/l - 72h (OECD Test Guideline 201)

Toxicity to bacteria: IC50 - Bacteria - 29 mg/l - 15h

Remarks: (ECHA)

**sec-Butyllithium**
No data available

---

**SECTION 13: Disposal considerations**

**13.1 Waste treatment methods**

**Product**
Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

---

**SECTION 14: Transport information**

**DOT (US)**
UN number: 3394  Class: 4.2 (4.3)  Packing group: I
Proper shipping name: Organometallic substance, liquid, pyrophoric, water-reactive (sec-Butyllithium, Cyclohexane)
Reportable Quantity (RQ): 1111 lbs
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 (Cyclohexane, sec-Butyllithium)
Marine pollutant: yes

**IATA**
UN number: 3394  Class: 4.2 (4.3)
Proper shipping name: Organometallic substance, liquid, pyrophoric, water-reactive (Cyclohexane, sec-Butyllithium)
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport
### SECTION 15: Regulatory information

**SARA 302 Components**
This material does not contain any components with a section 302 EHS TPQ.

**SARA 313 Components**
The following components are subject to reporting levels established by SARA Title III, Section 313:

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cyclohexane</td>
<td>110-82-7</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

**SARA 311/312 Hazards**
Fire Hazard, Reactivity Hazard, Acute Health Hazard, Chronic Health Hazard

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
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</thead>
<tbody>
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<td>Cyclohexane</td>
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</table>

**Pennsylvania Right To Know Components**

<table>
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<tbody>
<tr>
<td>Cyclohexane</td>
<td>110-82-7</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

### SECTION 16: Other information

**Further information**
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Version: 6.7      Revision Date: 05/24/2023      Print Date: 08/12/2023