

# SAFETY DATA SHEET

Version 6.7  
Revision Date 08/05/2024  
Print Date 08/06/2024

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

### 1.1 Product identifiers

Product name : Allyl hexanoate

Product Number : W203203

Brand : Aldrich

CAS-No. : 123-68-2

### 1.2 Relevant identified uses of the substance or mixture and uses advised against

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 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 4), H227

Acute toxicity, Oral (Category 3), H301

Acute toxicity, Dermal (Category 3), H311

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 Statements

H227

Combustible liquid.

H301 + H311

Toxic if swallowed or in contact with skin.

H411

Toxic to aquatic life with long lasting effects.

Precautionary Statements

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P273

Avoid release to the environment.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P310 + P330

IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.

P302 + P352 + P312

IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

P362

Take off contaminated clothing and wash before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P391

Collect spillage.

P403 + P235

Store in a well-ventilated place. Keep cool.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

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

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : Allyl caproate

Formula : C<sub>9</sub>H<sub>16</sub>O<sub>2</sub>

Molecular weight : 156.22 g/mol

CAS-No. : 123-68-2

EC-No. : 204-642-4

Component	Classification	Concentration
<b>Allyl hexanoate</b>	Flam. Liq. 4; Acute Tox. 3; Aquatic Acute 2; Aquatic Chronic 2; H227, H301,	<= 100 %

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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**

No data available

**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 (CO<sub>2</sub>) Foam Dry powder

**Unsuitable extinguishing media**

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides  
Combustible.

**5.3 Advice for firefighters**

No data available

**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**

For personal protection see section 8.

**6.2 Environmental precautions**

No data available

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

No data available

**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

For precautions see section 2.2.

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

No data available

### 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

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Personal protective equipment

##### Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 10 min

Material tested: Butoject® (KCL 898)

##### Control of environmental exposure

Prevent product from entering drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                                 |  |
|---------------------------------|--|
| a) Appearance                   | Form: liquid<br>Color: colorless         |
| 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        | 75 - 76 °C 167 - 169 °F at 20 hPa - lit. |

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- and boiling range
- g) Flash point 66 °C (151 °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 0.887 g/cm<sup>3</sup> at 25 °C (77 °F) - lit.  
Relative density No data available
  - n) Water solubility slightly soluble
  - o) Partition coefficient: n-octanol/water log Pow: 3.2 - Bioaccumulation is not expected.
  - p) Autoignition temperature No data available
  - q) Decomposition temperature No data available
  - r) Viscosity No data available
  - s) Explosive properties No data available
  - t) Oxidizing properties No data available

## 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

No data available

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:  
bases

### 10.4 Conditions to avoid

No data available

### 10.5 Incompatible materials

no information available

## 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

#### Acute toxicity

LD50 Oral - Rat - 218 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity).

Inhalation: No data available

LD50 Dermal - Rabbit - 300 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Human

#### 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

RTECS: MO6125000

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

Stomach - Irregularities - Based on Human Evidence

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 2.0 mg/l - 96.0 h  
Toxicity to daphnia and other aquatic invertebrates EC50 - Daphnia magna (Water flea) - 2 mg/l - 48 h

### 12.2 Persistence and degradability

Biodegradability Result: - According to the results of tests of biodegradability this product is not readily biodegradable.

### 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

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

No data available

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## SECTION 14: Transport information

### DOT (US)

UN number: 2810 Class: 6.1 Packing group: III  
Proper shipping name: Toxic, liquids, organic, n.o.s. (Allyl hexanoate)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

### IMDG

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UN number: 2810 Class: 6.1 Packing group: III EMS-No: F-A, S-A  
Proper shipping name: TOXIC LIQUID, ORGANIC, N.O.S. (Allyl hexanoate)  
Marine pollutant : yes

**IATA**

UN number: 2810 Class: 6.1 Packing group: III  
Proper shipping name: Toxic liquid, organic, n.o.s. (Allyl hexanoate)

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**SECTION 15: Regulatory information**

**CERCLA Reportable Quantity**

This material does not contain any components with a CERCLA RQ.

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

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

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**SARA 313** : 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.

**US State Regulations**

**Massachusetts Right To Know**

No components are subject to the Massachusetts Right to Know Act.

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.



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**SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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