

## Chemical Safety Data Sheet MSDS / SDS

## Allyl hexanoate

Revision Date:2026-05-31 Revision Number:1

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

## Product identifier

Product name : Allyl hexanoate  
CBnumber : CB9205910  
CAS : 123-68-2  
EINECS Number : 204-642-4  
Synonyms : ALLYL CAPROATE, ALLYL HEXANOATE

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

## Company Identification

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

## SECTION 2: Hazards identification

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

## Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.  
P264 Wash hands thoroughly after handling.  
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/protective clothing/eye protection/face protection.  
P312 Call a POISON CENTER or doctor/physician if you feel unwell.  
P370+P378 In case of fire: Use ... for extinction.  
P391 Collect spillage. Hazardous to the aquatic environment  
P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

P501 Dispose of contents/container to.....

#### **Hazard statements**

H227 Combustible liquid

H411 Toxic to aquatic life with long lasting effects

---

## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: Allyl hexanoate
Synonyms	: ALLYL CAPROATE, ALLYL HEXANOATE
CAS	: 123-68-2
EC number	: 204-642-4
MF	: C9H16O2
MW	: 156.22

---

## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General advice**

Consult a physician. Show this material safety data sheet to the doctor in attendance.

#### **If inhaled**

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

#### **In case of skin contact**

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

#### **In case of eye contact**

Flush eyes with water as a precaution.

#### **If swallowed**

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

### **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

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

No data available

---

## SECTION 5: Firefighting measures

### **Extinguishing media**

#### **Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### Unsuitable extinguishing media

Do NOT use water jet.

### Special hazards arising from the substance or mixture

Carbon oxides

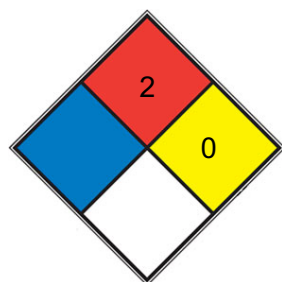
### Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### Further information

Use water spray to cool unopened containers.

### NFPA 704



■ HEALTH

Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely

■ FIRE 2 divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, [sulfur](#))

■ REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

□ SPEC.

□ HAZ.

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. 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.

### 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.

### Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13). Keep in suitable, closed containers for disposal.

### Reference to other sections

For disposal see section 13.

---

## SECTION 7: Handling and storage

### Precautions for safe handling

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

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

For precautions see section 2.2.

### Conditions for safe storage, including any incompatibilities

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. Store in cool place.

### 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

### control parameter

#### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

### Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses 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.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 156 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

Complete suit protecting against chemicals, 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.

---

## SECTION 9: Physical and chemical properties

### Information on basic physicochemical properties

Appearance	colorless liquid
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	-57.45°C (estimate)
Initial boiling point and boiling range	75 - 76 °C at 20 hPa - lit.
Flash point	66 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	No data available
Vapour pressure	No data available
Vapour density	No data available
Relative density	0,887 g/cm <sup>3</sup> at 25 °C
Water solubility	0.06g/l
Partition coefficient: n-octanol/water	log Pow: 3,2
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

### Other safety information

No data available

---

## SECTION 10: Stability and reactivity

### Reactivity

No data available

### **Chemical stability**

Stable under recommended storage conditions.

### **Possibility of hazardous reactions**

No data available

### **Conditions to avoid**

Heat, flames and sparks.

### **Incompatible materials**

Strong oxidizing agents

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available

In the event of fire: see section 5

---

## **SECTION 11: Toxicological information**

### **Information on toxicological effects**

#### **Acute toxicity**

LD50 Oral - Rat - 218 mg/kg

Remarks: Behavioral:Somnolence (general depressed activity). LD50 Dermal - Rabbit - 300 mg/kg

#### **Skin corrosion/irritation**

Skin - Human

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

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.

#### **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

#### **Additional Information**

RTECS: MO6125000

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

#### **toxicity**

The acute oral LD<sub>50</sub> in rats was 218 mg/kg and in guinea-pigs 280 mg/kg . The acute dermal LD<sub>50</sub> for sample no. 71-20 was reported as 0-3ml/kg in the rabbit

---

## SECTION 12: Ecological information

### **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

### **Persistence and degradability**

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

### **Bioaccumulative potential**

No data available

### **Mobility in soil**

No data available

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

### **Other adverse effects**

Toxic to aquatic life with long lasting effects.

---

## SECTION 13: Disposal considerations

### **Waste treatment methods**

#### **Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

#### **Contaminated packaging**

Dispose of as unused product.

---

## SECTION 14: Transport information

### UN number

ADR/RID: 2810 IMDG: 2810 IATA: 2810

### UN proper shipping name

ADR/RID: TOXIC LIQUID, ORGANIC, N.O.S. (Allyl hexanoate) IMDG: TOXIC LIQUID,  
ORGANIC, N.O.S. (Allyl hexanoate)

IATA: Toxic liquid, organic, n.o.s. (Allyl  
hexanoate)

14.3	Transport hazard class(es) ADR/RID: 6.1 IMDG: 6.1	IATA: 6.1
14.4	Packaging group ADR/RID: III IMDG: III	IATA: III
14.5	Environmental hazards ADR/RID: yes IMDG Marine pollutant: yes	IATA: no
14.6	Special precautions for user No data available	

---

## SECTION 15: Regulatory information

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

#### Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

---

## SECTION 16: Other information

### Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.