

SAFETY DATA SHEET

Version 5.3
Revision Date 07/09/2014
Print Date 11/10/2018

1. PRODUCT AND COMPANY IDENTIFICATION

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, Manufacture of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832
Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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
Acute aquatic toxicity (Category 2), H401
Chronic aquatic toxicity (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)

H227 : Combustible liquid
H301 + H311 : Toxic if swallowed or in contact with skin
H411 : Toxic to aquatic life with long lasting effects.

Precautionary statement(s)

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/ protective clothing/ eye protection/ face protection.

P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P312	Call a POISON CENTER or doctor/ physician if you feel unwell.
P322	Specific measures (see supplemental first aid instructions on this label).
P330	Rinse mouth.
P361	Remove/Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms	: Allyl caproate
Formula	: C ₉ H ₁₆ O ₂
Molecular Weight	: 156.22 g/mol
CAS-No.	: 123-68-2
EC-No.	: 204-642-4

Hazardous components

Component	Classification	Concentration
Allyl hexanoate		
	Flam. Liq. 4; Acute Tox. 3; Aquatic Acute 2; Aquatic Chronic 2; H227, H301 + H311, H411	90 - 100 %

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this 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

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.

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

5. FIREFIGHTING MEASURES

5.1 Extinguishing media

Suitable extinguishing media

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

5.2 Special hazards arising from the substance or mixture

Carbon oxides

5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES

6.1 Personal precautions, protective equipment and emergency procedures

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations.

Vapours 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). Keep in suitable, closed containers for disposal.

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE

7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapour 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.

7.2 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.

7.3 Specific end use(s)

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

8. EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1 Control parameters

Components with workplace control parameters

Contains no substances with occupational exposure limit values.

8.2 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.

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 CE 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.

9. PHYSICAL AND CHEMICAL PROPERTIES**9.1 Information on basic physical and chemical properties**

- | | |
|---|--|
| a) Appearance | Form: liquid
Colour: colourless |
| b) Odour | no data available |
| c) Odour Threshold | no data available |
| d) pH | no data available |
| e) Melting point/freezing point | no data available |
| f) Initial boiling point and boiling range | 75 - 76 °C (167 - 169 °F) at 20 hPa (15 mmHg) - lit. |
| 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) Vapour pressure | no data available |
| l) Vapour density | no data available |
| m) Relative density | 0.887 g/cm ³ at 25 °C (77 °F) |
| n) Water solubility | no data available |
| o) Partition coefficient: n-octanol/water | log Pow: 3.2 |

- p) Auto-ignition 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

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

no data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

Other decomposition products - no data available
In the event of fire: see section 5

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

no data available

Respiratory or skin sensitisation

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

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

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

NTP: No component 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 identified as a carcinogen or potential carcinogen by OSHA.

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

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

Stomach - Irregularities - Based on Human Evidence

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 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.
Toxic to aquatic life with long lasting effects.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. 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.

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):
Marine pollutant: No
Poison Inhalation Hazard: No

IMDG

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: Marine pollutant

IATA

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

15. REGULATORY INFORMATION

SARA 302 Components

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

SARA 313 Components

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.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Allyl hexanoate	123-68-2	

New Jersey Right To Know Components

	CAS-No.	Revision Date
Allyl hexanoate	123-68-2	

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3.

Acute Tox.	Acute toxicity
Aquatic Acute	Acute aquatic toxicity
Aquatic Chronic	Chronic aquatic toxicity
Flam. Liq.	Flammable liquids
H227	Combustible liquid
H301	Toxic if swallowed.
H301 + H311	Toxic if swallowed or in contact with skin

HMIS Rating

Health hazard:	2
Chronic Health Hazard:	
Flammability:	2
Physical Hazard	0

NFPA Rating

Health hazard:	2
Fire Hazard:	2
Reactivity Hazard:	0

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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