

SAFETY DATA SHEET

Version 6.4
Revision Date 01/08/2022
Print Date 02/05/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Allyl cyclohexanepropionate

Product Number : 18018
Brand : Sigma-Aldrich
CAS-No. : 2705-87-5

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)**

Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Skin sensitization (Category 1), H317
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

Pictogram



Signal word

Warning

Hazard statement(s)	
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H317	May cause an allergic skin reaction.
H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing must not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of water.Call a POISON CENTER/ doctor if you feel unwell.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P363	Wash contaminated clothing before reuse.
P391	Collect spillage.
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	: Cyclohexanepropanoic acid 2-propen-1-yl ester Cyclohexanepropionic acid allyl ester 2-Propenyl 3-cyclohexylpropanoate
Formula	: C ₁₂ H ₂₀ O ₂
Molecular weight	: 196.29 g/mol
CAS-No.	: 2705-87-5
EC-No.	: 220-292-5

Component	Classification	Concentration
Allyl 3-cyclohexylpropionate		
	Acute Tox. 4; Skin Sens. 1; Aquatic Acute 1; Aquatic Chronic 1; H302, H332, H312, H317, H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	<= 100 %

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

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

If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

In case of skin contact

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

In case of eye contact

After eye contact: rinse out with plenty of water. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Foam Carbon dioxide (CO₂) 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.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

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

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. 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.

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 with liquid-absorbent material (e.g. Chemisorb®). 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.

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.

Storage class

Storage class (TRGS 510): 10: Combustible liquids

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

Contains no substances with occupational exposure limit values.

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). Safety glasses

Skin protection

required

Body Protection

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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: colorless
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Freezing point: < -20 °C (< -4 °F) at 1,013 hPa - OECD Test Guideline 102
f) Initial boiling point and boiling range	266.3 °C 511.3 °F at 1,013 hPa - OECD Test Guideline 103 91 °C (196 °F) at 1 hPa
g) Flash point	106 °C (223 °F) - closed cup - Regulation (EC) No. 440/2008, Annex, A.9
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	0.0 hPa at 25 °C (77 °F) - OECD Test Guideline 104
l) Vapor density	No data available
m) Density	0.948 g/cm ³
Relative density	No data available
n) Water solubility	0.017 g/l at 20 °C (68 °F) - OECD Test Guideline 105
o) Partition coefficient: n-octanol/water	log Pow: 4.28 at 20 °C (68 °F) - OECD Test Guideline 107 - Potential bioaccumulation

Sigma-Aldrich - 18018

Page 5 of 10

- | | |
|------------------------------|-------------------|
| 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 | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Forms explosive mixtures with air on intense heating.
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Strong heating.

10.5 Incompatible materials

Strong oxidizing agents

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - 585 mg/kg
(OECD Test Guideline 401)

Acute toxicity estimate Inhalation - 4 h - 11.1 mg/l - vapor

(Expert judgment)

LD50 Dermal - Rabbit - 1,600 mg/kg
(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - reconstructed human epidermis (RhE)

Result: No skin irritation
(OECD Test Guideline 439)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Germ cell mutagenicity

Test Type: in vitro test

Test system: human lymphoblastoid cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 487

Result: negative

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster fibroblasts

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

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

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: GV6735000

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	flow-through test LC50 - <i>Pimephales promelas</i> (fathead minnow) - 0.13 mg/l - 96 h
------------------	---

Sigma-Aldrich - 18018

Page 7 of 10

	(OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	flow-through test EC50 - Daphnia magna (Water flea) - 3.8 mg/l - 48 h (OECD Test Guideline 202)
	flow-through test NOEC - Daphnia magna (Water flea) - 0.86 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 3 mg/l - 72 h (OECD Test Guideline 201)
	static test NOEC - Pseudokirchneriella subcapitata (green algae) - 0.74 mg/l - 72 h (OECD Test Guideline 201)

12.2 Persistence and degradability

Biodegradability aerobic - Exposure time 28 d
Result: 86 % - Readily biodegradable.
(OECD Test Guideline 301D)

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

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)

Not dangerous goods

IMDG

UN number: 3082 Class: 9

Packing group: III

EMS-No: F-A, S-F

Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (Allyl 3-cyclohexylpropionate)
Marine pollutant : yes

IATA

UN number: 3082 Class: 9 Packing group: III
Proper shipping name: Environmentally hazardous substance, liquid, n.o.s. (Allyl 3-cyclohexylpropionate)

Further information

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

SECTION 15: Regulatory information

SARA 302 Components

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

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

Acute Health Hazard

Massachusetts Right To Know Components

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

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

Pennsylvania Right To Know Components

Allyl 3-cyclohexylpropionate	CAS-No. 2705-87-5	Revision Date
------------------------------	----------------------	---------------

New Jersey Right To Know Components

Allyl 3-cyclohexylpropionate	CAS-No. 2705-87-5	Revision Date
------------------------------	----------------------	---------------

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

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.

Version: 6.4

Revision Date: 01/08/2022

Print Date: 02/05/2022