

# safety data sheet

according to Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU



## Allyl caproate ROTICHROM® GC

article number: **3792**  
Version: **1.0 en**

date of compilation: 2016-03-04

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

#### 1.1 Product identifier

Identification of the substance	<b>Allyl caproate</b>
Article number	3792
Registration number (REACH)	This information is not available.
EC number	204-642-4
CAS number	123-68-2

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

**Identified uses:** laboratory chemical

#### 1.3 Details of the supplier of the safety data sheet

Carl Roth GmbH + Co KG  
Schoemperlenstr. 3-5  
D-76185 Karlsruhe  
Germany

**Telephone:** +49 (0) 721 - 56 06 0

**Telefax:** +49 (0) 721 - 56 06 149

**e-mail:** [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

**Website:** [www.carlroth.de](http://www.carlroth.de)

Competent person responsible for the safety data sheet : Department Health, Safety and Environment

**e-mail (competent person)** : [sicherheit@carlroth.de](mailto:sicherheit@carlroth.de)

#### 1.4 Emergency telephone number

Emergency information service **Poison Centre Munich: +49/(0)89 19240**

### SECTION 2: Hazards identification

#### 2.1 Classification of the substance or mixture

**Classification according to Regulation (EC) No 1272/2008 (CLP)**

Classification acc. to GHS			
Section	Hazard class	Hazard class and category	Hazard statement
3.1O	acute toxicity (oral)	(Acute Tox. 3)	H301
3.1D	acute toxicity (dermal)	(Acute Tox. 3)	H311
4.1C	hazardous to the aquatic environment - chronic hazard	(Aquatic Chronic 2)	H411

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### Remarks

For full text of Hazard- and EU Hazard-statements: see SECTION 16.

## 2.2 Label elements

### Labelling according to Regulation (EC) No 1272/2008 (CLP)

#### Signal word

**Danger**

#### Pictograms



#### Hazard statements

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

#### Precautionary statements

##### Precautionary statements - prevention

P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing.

##### Precautionary statements - response

P302+P352 IF ON SKIN: Wash with plenty of soap and water.  
P312 Call a POISON CENTER/doctor if you feel unwell.

#### Labelling of packages where the contents do not exceed 125 ml

Signal word: **Danger**

Symbol(s)



H301+H311 Toxic if swallowed or in contact with skin.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P302+P352 IF ON SKIN: Wash with plenty of water.  
P312 Call a POISON CENTER/doctor if you feel unwell.

## 2.3 Other hazards

There is no additional information.

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### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Name of substance	Allyl caproate
EC number	204-642-4
CAS number	123-68-2
Molecular formula	C <sub>9</sub> H <sub>16</sub> O <sub>2</sub>
Molar mass	156,2 g/mol

### SECTION 4: First aid measures

#### 4.1 Description of first aid measures



##### General notes

Take off immediately all contaminated clothing. Self-protection of the first aider.

##### Following inhalation

Provide fresh air. In all cases of doubt, or when symptoms persist, seek medical advice.

##### Following skin contact

After contact with skin, wash immediately with plenty of water.

##### Following eye contact

Rinse cautiously with water for several minutes. In all cases of doubt, or when symptoms persist, seek medical advice.

##### Following ingestion

Rinse mouth immediately and drink plenty of water. Call a physician immediately.

#### 4.2 Most important symptoms and effects, both acute and delayed

Dizziness, Irritant effects

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

none

### SECTION 5: Firefighting measures

#### 5.1 Extinguishing media

##### Suitable extinguishing media

Co-ordinate fire-fighting measures to the fire surroundings  
foam, dry extinguishing powder, carbon dioxide (CO<sub>2</sub>)

##### Unsuitable extinguishing media

water jet

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

Combustible.

#### Hazardous combustion products

In case of fire may be liberated: carbon monoxide (CO), carbon dioxide (CO<sub>2</sub>)

### 5.3 Advice for firefighters

Do not allow firefighting water to enter drains or water courses. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus. Wear full chemical protective clothing.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

#### For non-emergency personnel

Wearing of suitable protective equipment (including personal protective equipment referred to under Section 8 of the safety data sheet) to prevent any contamination of skin, eyes and personal clothing. Avoid contact with skin, eyes and clothes. Do not breathe vapour/spray.

### 6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose it.

### 6.3 Methods and material for containment and cleaning up

#### Advices on how to contain a spill

Covering of drains.

#### Advices on how to clean up a spill

Absorb with liquid-binding material (e.g. sand, diatomaceous earth, acid- or universal binding agents).

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

#### Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Provision of sufficient ventilation. Handle and open container with care.

#### • Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

#### Advice on general occupational hygiene

When using do not eat or drink. Thorough skin-cleansing after handling the product.

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

Keep container tightly closed in a cool place.

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### Incompatible substances or mixtures

Observe hints for combined storage.

### Consideration of other advice

Store locked up.

#### • Ventilation requirements

Use local and general ventilation.

#### • Specific designs for storage rooms or vessels

Recommended storage temperature: 4 °C.

### 7.3 Specific end use(s)

No information available.

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### National limit values

#### Occupational exposure limit values (Workplace Exposure Limits)

No data available.

### 8.2 Exposure controls

#### Individual protection measures (personal protective equipment)



#### Eye/face protection

Use safety goggle with side protection.

#### Skin protection

##### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

##### • type of material

Butyl caoutchouc (butyl rubber)

##### • material thickness

0,7mm.

##### • breakthrough times of the glove material

>10 minutes (permeation: level 1)

##### • other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended.

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### Respiratory protection

Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of > 65 °C, colour code: Brown).

Observe the wear time limits according GefStoffV in combination with the rules for using respiratory protection apparatus (BGR 190).

### Environmental exposure controls

Keep away from drains, surface and ground water.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

#### Appearance

Physical state	liquid (fluid)
Colour	this information is not available
Odour	fruity
Odour threshold	No data available

#### Other physical and chemical parameters

pH (value)	This information is not available.
Melting point/freezing point	not determined
Initial boiling point and boiling range	186 - 191 °C
Flash point	74 °C (closed cup)
Evaporation rate	no data available
Flammability (solid, gas)	not relevant (fluid)
<u>Explosive limits</u>	
• lower explosion limit (LEL)	this information is not available
• upper explosion limit (UEL)	this information is not available
Explosion limits of dust clouds	not relevant
Vapour pressure	This information is not available.
Density	0,887 g/cm <sup>3</sup> at 25 °C
Vapour density	This information is not available.
Bulk density	Not applicable
Relative density	Information on this property is not available.
<u>Solubility(ies)</u>	
Water solubility	0,06 g/l at 20 °C
<u>Partition coefficient</u>	
n-octanol/water (log KOW)	3,2 (calculated value)
Auto-ignition temperature	Information on this property is not available.
Decomposition temperature	no data available
Viscosity	not determined
Explosive properties	none

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Oxidising properties none

### 9.2 Other information

Refractive index 1,425

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

In case of warming: Vapours can form explosive mixtures with air.

### 10.2 Chemical stability

The material is stable under normal ambient and anticipated storage and handling conditions of temperature and pressure.

### 10.3 Possibility of hazardous reactions

Violent reaction with: Alkalis

### 10.4 Conditions to avoid

There are no specific conditions known which have to be avoided.

### 10.5 Incompatible materials

There is no additional information.

### 10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

Exposure route	Endpoint	Value	Species	Source
oral	LD50	218 mg/kg	rat	TOXNET
dermal	LD50	300 mg/kg	rabbit	TOXNET

#### Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

#### Serious eye damage/eye irritation

Shall not be classified as seriously damaging to the eye or eye irritant.

#### Respiratory or skin sensitisation

Shall not be classified as a respiratory or skin sensitiser.

#### Summary of evaluation of the CMR properties

Shall not be classified as germ cell mutagenic, carcinogenic nor as a reproductive toxicant

- **Specific target organ toxicity - single exposure**

Shall not be classified as a specific target organ toxicant (single exposure).

- **Specific target organ toxicity - repeated exposure**

Shall not be classified as a specific target organ toxicant (repeated exposure).

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### Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

### Symptoms related to the physical, chemical and toxicological characteristics

- **If swallowed**

data are not available

- **If in eyes**

data are not available

- **If inhaled**

data are not available

- **If on skin**

data are not available

### Other information

Dizziness

## SECTION 12: Ecological information

### 12.1 Toxicity

Toxic to aquatic life with long lasting effects.

#### Aquatic toxicity (acute)

Endpoint	Value	Species	Source	Exposure time
EC50	2 mg/l	daphnia magna		48 hours
LC50	30 mg/l	goldfish (Carassius auratus)		96 hours
LC50	2 mg/l	Pimephales promelas		96 hours

#### Aquatic toxicity (chronic)

May cause long-term adverse effects in the aquatic environment.

### 12.2 Process of degradability

Not readily biodegradable.

Theoretical Oxygen Demand: 2,458 mg/mg

Theoretical Carbon Dioxide: 2,535 mg/mg

### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)

3,2

### 12.4 Mobility in soil

Data are not available.

### 12.5 Results of PBT and vPvB assessment

Data are not available.

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### 12.6 Other adverse effects

Hazardous to water.

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

This material and its container must be disposed of as hazardous waste. Dispose of contents/container in accordance with local/regional/national/international regulations.

#### Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

#### Waste treatment of containers/packagings

It is a dangerous waste; only packagings which are approved (e.g. acc. to ADR) may be used.

### 13.2 Relevant provisions relating to waste

The allocation of waste identity numbers/waste descriptions must be carried out according to the EEC, specific to the industry and process.

### 13.3 Remarks

Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities. Please consider the relevant national or regional provisions.

## SECTION 14: Transport information

14.1	UN number	2810
14.2	UN proper shipping name	TOXIC LIQUID, ORGANIC, N.O.S.
	Hazardous ingredients	Allyl caproate
14.3	Transport hazard class(es)	
	Class	6.1 (toxic substances)
14.4	Packing group	III (substance presenting low danger)
14.5	Environmental hazards	hazardous to the aquatic environment

### 14.6 Special precautions for user

Provisions for dangerous goods (ADR) should be complied within the premises.

### 14.7 Transport in bulk according to Annex II of MARPOL and the IBC Code

The cargo is not intended to be carried in bulk.

### 14.8 Information for each of the UN Model Regulations

#### • Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN)

UN number	2810
Proper shipping name	TOXIC LIQUID, ORGANIC, N.O.S.
Particulars in the transport document	UN2810, TOXIC LIQUID, ORGANIC, N.O.S., (allyl hexanoate), 6.1, III, (E), environmentally hazardous
Class	6.1
Classification code	T1
Packing group	III
Danger label(s)	6.1 + "fish and tree"

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Environmental hazards	yes (hazardous to the aquatic environment)
Special provisions (SP)	274, 614, 802(ADN)
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
Transport category (TC)	2
Tunnel restriction code (TRC)	E
Hazard identification No	60
<b>Emergency Action Code</b>	2X
<b>• International Maritime Dangerous Goods Code (IMDG)</b>	
UN number	2810
Proper shipping name	TOXIC LIQUID, ORGANIC, N.O.S.
Particulars in the shipper's declaration	UN2810, TOXIC LIQUID, ORGANIC, N.O.S., (allyl hexanoate), 6.1, III, MARINE POLLUTANT
Class	6.1
Marine pollutant	yes (hazardous to the aquatic environment)
Packing group	III
Danger label(s)	6.1 + "fish and tree"
Special provisions (SP)	223, 274
Excepted quantities (EQ)	E1
Limited quantities (LQ)	5 L
EmS	F-A, S-A
Stowage category	B

## SECTION 15: Regulatory information

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

#### Relevant provisions of the European Union (EU)

- Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)  
Not listed.

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- **Regulation 1005/2009/EC on substances that deplete the ozone layer (ODS)**

Not listed.

- **Regulation 850/2004/EC on persistent organic pollutants (POP)**

Not listed.

- **Restrictions according to REACH, Annex XVII**

not listed

- **List of substances subject to authorisation (REACH, Annex XIV)**

not listed

- **Seveso Directive**

2012/18/EU (Seveso III)				
No	Dangerous substance/hazard categories	Qualifying quantity (tonnes) for the application of lower and upper-tier requirements		Notes
E2	environmental hazards (hazardous to the aquatic environment, cat. 2)	200	500	57)

**Notation**

57) Hazardous to the Aquatic Environment in category Chronic 2

- **Limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products (2004/42/EC, Deco-Paint Directive)**

VOC content 100 %

- **Directive on industrial emissions (VOCs, 2010/75/EU)**

VOC content 100 %

- **Directive 2011/65/EU on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS) - Annex II**

not listed

- **Regulation 166/2006/EC concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)**

not listed

- **Directive 2000/60/EC establishing a framework for Community action in the field of water policy (WFD)**

not listed

### National inventories

Substance is listed in the following national inventories:

- EINECS/ELINCS/NLP (Europe)
- REACH (Europe)

## 15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

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### SECTION 16: Other information

#### Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de navigation intérieures (European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
CMR	Carcinogenic, Mutagenic or toxic for Reproduction
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IMDG	International Maritime Dangerous Goods Code
MARPOL	International Convention for the Prevention of Pollution from Ships (abbr. of "Marine Pollutant")
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
REACH	Registration, Evaluation, Authorisation and Restriction of Chemicals
RID	Règlement concernant le transport International ferroviaire des marchandises Dangereuses (Regulations concerning the International carriage of Dangerous goods by Rail)
VOC	Volatile Organic Compounds
vPvB	very Persistent and very Bioaccumulative

#### Key literature references and sources for data

- Regulation (EC) No. 1907/2006 (REACH), amended by 2015/830/EU
- Regulation (EC) No. 1272/2008 (CLP, EU GHS)

#### List of relevant phrases (code and full text as stated in chapter 2 and 3)

Code	Text
H301	toxic if swallowed
H311	toxic in contact with skin
H411	toxic to aquatic life with long lasting effects

#### Disclaimer

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.