

# Safety data sheet

acc. to Regulation (EC) No. 1907/2006 (REACH)



## Caprylic acid methyl ester $\geq 99\%$ , for synthesis

article number: **3331**  
Version: **3.0 en**  
Replaces version of: 2021-12-03  
Version: (2)

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

### 1.1 Product identifier

Identification of the substance	<b>Caprylic acid methyl ester <math>\geq 99\%</math>, for synthesis</b>
Article number	3331
EC number	203-835-0
CAS number	111-11-5

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

Relevant identified uses:	Laboratory chemical Laboratory and analytical use
Uses advised against:	Do not use for private purposes (household). Food, drink and animal feedingstuffs.

### 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

Name	Street	Postal code/city	Telephone	Website
National Poisons Information Service City Hospital	Dudley Rd	B187QH Birmingham	844 892 0111	

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Classification acc. to GHS

Section	Hazard class	Cat-egory	Hazard class and category	Hazard statement
3.2	Skin corrosion/irritation	2	Skin Irrit. 2	H315

For full text of abbreviations: see SECTION 16

### 2.2 Label elements

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### Labelling

#### Signal word

Warning

#### Pictograms

GHS07



#### Hazard statements

H315

Causes skin irritation

#### Precautionary statements

##### Precautionary statements - prevention

P280

Wear protective gloves/eye protection

##### Precautionary statements - response

P302+P352

IF ON SKIN: Wash with plenty of soap and water

P332+P313

If skin irritation occurs: Get medical advice/attention

### 2.3 Other hazards

This material is combustible, but will not ignite readily.

#### Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

#### Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Name of substance	Caprylic acid methyl ester
Molecular formula	$C_9H_{18}O_2$
Molar mass	158,2 g/mol
CAS No	111-11-5
EC No	203-835-0

## SECTION 4: First aid measures

### 4.1 Description of first aid measures



#### General notes

Take off contaminated clothing.

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### Following inhalation

Provide fresh air.

### Following skin contact

Rinse skin with water/shower. In case of skin irritation, consult a physician.

### Following eye contact

Rinse cautiously with water for several minutes.

### Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

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

Irritation

## 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 firefighting measures to the fire surroundings!  
water spray, dry extinguishing powder, BC-powder, carbon dioxide (CO<sub>2</sub>)

#### Unsuitable extinguishing media

water jet

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

Combustible. Vapours are heavier than air, spread along floors and form explosive mixtures with air.

#### Hazardous combustion products

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

### 5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Fight fire with normal precautions from a reasonable distance. Wear self-contained breathing apparatus.

## SECTION 6: Accidental release measures

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



#### For non-emergency personnel

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 of it.

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

#### Advice on how to contain a spill

Covering of drains.

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

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

#### Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

### 6.4 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.

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



Keep away from sources of ignition - No smoking.

#### Advice on general occupational hygiene

Wash hands before breaks and after work. Keep away from food, drink and animal feedingstuffs.

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

Keep in a cool place.

#### Incompatible substances or mixtures

Observe hints for combined storage.

#### Consideration of other advice:

#### Specific designs for storage rooms or vessels

Recommended storage temperature: 2 – 8 °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)

This information is not available.

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### Environmental values

Relevant PNECs and other threshold levels				
End-point	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	0,048 mg/l	aquatic organisms	water	intermittent release
PNEC	0,002 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	0 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	100 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,028 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,003 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	10 mg/kg	terrestrial organisms	soil	short-term (single instance)

## 8.2 Exposure controls

### Individual protection measures (personal protective equipment)

#### Eye/face protection



Use safety goggles with side protection.

#### Skin protection



#### • hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. 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. The times are approximate values from measurements at 22 ° C and permanent contact. Increased temperatures due to heated substances, body heat etc. and a reduction of the effective layer thickness by stretching can lead to a considerable reduction of the breakthrough time. If in doubt, contact manufacturer. At an approx. 1.5 times larger / smaller layer thickness, the respective breakthrough time is doubled / halved. The data apply only to the pure substance. When transferred to substance mixtures, they may only be considered as a guide.

#### • type of material

NBR (Nitrile rubber)

#### • material thickness

>0,11 mm

#### • breakthrough times of the glove material

>480 minutes (permeation: level 6)

#### • other protection measures

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

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recommended.

### Respiratory protection



Respiratory protection necessary at: Aerosol or mist formation. Type: A (against organic gases and vapours with a boiling point of  $> 65\text{ }^{\circ}\text{C}$ , colour code: Brown).

### 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

Physical state	liquid
Colour	colourless - clear
Odour	fruity
Melting point/freezing point	$-40\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Boiling point or initial boiling point and boiling range	$192,6\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Flammability	this material is combustible, but will not ignite readily
Lower and upper explosion limit	not determined
Flash point	$82\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Auto-ignition temperature	$290\text{ }^{\circ}\text{C}$ at 1.013 hPa (ECHA)
Decomposition temperature	not relevant
pH (value)	not determined
Kinematic viscosity	$1,6\text{ mm}^2/\text{s}$ at $20\text{ }^{\circ}\text{C}$
Dynamic viscosity	$1,403\text{ cP}$ at $20\text{ }^{\circ}\text{C}$
<u>Solubility(ies)</u>	
Water solubility	$0,064\text{ g/l}$ at $20\text{ }^{\circ}\text{C}$ (poorly soluble) (ECHA)
Solubility in alcohol	soluble
<u>Partition coefficient</u>	
Partition coefficient n-octanol/water (log value):	3,32 (ECHA)
Soil organic carbon/water (log KOC)	2,69 (ECHA)
<u>Vapour pressure</u>	
	$0,719\text{ hPa}$ at $25\text{ }^{\circ}\text{C}$ $1,33\text{ Pa}$ at $34,2\text{ }^{\circ}\text{C}$

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### Density and/or relative density

Density 0,877 g/cm<sup>3</sup> at 20 °C

Relative vapour density 5,45 (air = 1)

Particle characteristics not relevant (liquid)

### Other safety parameters

Oxidising properties none

## 9.2 Other information

Information with regard to physical hazard classes: hazard classes acc. to GHS (physical hazards): not relevant

Other safety characteristics:

Refractive index 1,417

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

This material is not reactive under normal ambient conditions.

#### **If heated**

Vapours may 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:** strong oxidiser

### 10.4 Conditions to avoid

Keep away from sources of ignition - No smoking.

### 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

#### **Classification acc. to GHS**

#### **Acute toxicity**

Shall not be classified as acutely toxic.

GHS of the United Nations, annex 4. May be harmful if swallowed.

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Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	$>2.000 \text{ mg/kg}$	rat		ECHA

### Skin corrosion/irritation

Causes skin irritation.

### 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.

### Germ cell mutagenicity

Shall not be classified as germ cell mutagenic.

### Carcinogenicity

Shall not be classified as carcinogenic.

### Reproductive toxicity

Shall not be classified 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).

### 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

causes skin irritation

#### • Other information

none

### 11.2 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

### 11.3 Information on other hazards

There is no additional information.



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### SECTION 12: Ecological information

#### 12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)				
Endpoint	Value	Species	Source	Exposure time
LC50	5,6 mg/l	aquatic invertebrates	ECHA	48 h
EC50	4,76 mg/l	algae	ECHA	96 h

  

Aquatic toxicity (chronic)				
Endpoint	Value	Species	Source	Exposure time
EC50	>1.000 mg/l	microorganisms	ECHA	3 h

#### 12.2 Persistence and degradability

Theoretical Oxygen Demand: 2,528 mg/mg  
Theoretical Carbon Dioxide: 2,503 mg/mg

##### Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
oxygen depletion	78 %	28 d

#### 12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

n-octanol/water (log KOW)	3,32 (ECHA)
---------------------------	-------------

#### 12.4 Mobility in soil

Henry's law constant	0,001 Pa m <sup>3</sup> /mol at 25 °C (ECHA)
The Organic Carbon normalised adsorption coefficient	2,69 (ECHA)

#### 12.5 Results of PBT and vPvB assessment

Data are not available.

#### 12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) at a concentration of  $\geq 0,1\%$ .

#### 12.7 Other adverse effects

Data are not available.

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### 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.

##### Waste treatment of containers/packagings

Handle contaminated packages in the same way as the substance itself. Completely emptied packages can be recycled.

#### 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.

##### Properties of waste which render it hazardous

**HP 4** irritant - skin irritation and eye damage

#### 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. Non-contaminated packages may be recycled.

### SECTION 14: Transport information

- |   |   |
|---|---|
| 14.1 UN number or ID number   | not subject to transport regulations                                  |
| 14.2 UN proper shipping name  | not assigned  |
| 14.3 Transport hazard class(es)   | none  |
| 14.4 Packing group  | not assigned  |
| 14.5 Environmental hazards  | non-environmentally hazardous acc. to the dangerous goods regulations |
| 14.6 Special precautions for user   | There is no additional information.                                   |
| 14.7 Maritime transport in bulk according to IMO instruments                              | The cargo is not intended to be carried in bulk.                      |
| 14.8 <u>Information for each of the UN Model Regulations</u>                              |   |
| <b>International Maritime Dangerous Goods Code (IMDG) - Additional information</b>        | Not subject to IMDG.  |
| <b>International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information</b> | Not subject to ICAO-IATA.   |

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## 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)

##### 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
	not assigned		

##### Deco-Paint Directive

VOC content	100 %
VOC content	877 g/l

##### Industrial Emissions Directive (IED)

VOC content	100 %
VOC content	877 g/l

##### Directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment (RoHS)

not listed

##### Regulation concerning the establishment of a European Pollutant Release and Transfer Register (PRTR)

not listed

##### Water Framework Directive (WFD)

not listed

##### Regulation on the marketing and use of explosives precursors

not listed

##### Regulation on drug precursors

not listed

##### Regulation on substances that deplete the ozone layer (ODS)

not listed

##### Regulation concerning the export and import of hazardous chemicals (PIC)

not listed

##### Regulation on persistent organic pollutants (POP)

not listed

##### National regulations(GB)

##### List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list

not listed

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### Restrictions according to GB REACH, Annex 17

Dangerous substances with restrictions (GB REACH, Annex 17)			
Name of substance	Name acc. to inventory	CAS No	No
Caprylic acid methyl ester	this product meets the criteria for classification in accordance with Regulation No 1272/2008/EC		3

### Other information

Directive 94/33/EC on the protection of young people at work. Observe employment restrictions under the Maternity Protection Directive (92/85/EEC) for expectant or nursing mothers.

### National inventories

Country	Inventory	Status
AU	AIIC	substance is listed
CA	DSL	substance is listed
CN	IECSC	substance is listed
EU	ECSI	substance is listed
EU	REACH Reg.	substance is listed
JP	CSCL-ENCS	substance is listed
KR	KECI	substance is listed
MX	INSQ	substance is listed
NZ	NZIoC	substance is listed
PH	PICCS	substance is listed
TW	TCSI	substance is listed
US	TSCA	substance is listed (ACTIVE)
VN	NCI	substance is listed

#### Legend

AIIC	Australian Inventory of Industrial Chemicals
CSCL-ENCS	List of Existing and New Chemical Substances (CSCL-ENCS)
DSL	Domestic Substances List (DSL)
ECSI	EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC	Inventory of Existing Chemical Substances Produced or Imported in China
INSQ	National Inventory of Chemical Substances
KECI	Korea Existing Chemicals Inventory
NCI	National Chemical Inventory
NZIoC	New Zealand Inventory of Chemicals
PICCS	Philippine Inventory of Chemicals and Chemical Substances (PICCS)
REACH Reg.	REACH registered substances
TCSI	Taiwan Chemical Substance Inventory
TSCA	Toxic Substance Control Act

## 15.2 Chemical safety assessment

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

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### SECTION 16: Other information

#### Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
2.2	Labelling of packages where the contents do not exceed 125 ml: Signal word: Warning		yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.2		Labelling of packages where the contents do not exceed 125 ml: change in the listing (table)	yes
2.3		Endocrine disrupting properties: Does not contain an endocrine disruptor (ED) at a concentration of $\geq 0,1\%$ .	yes
14.8	Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information: Not subject to ADR, RID and ADN.		yes
15.1	Restrictions according to REACH, Annex XVII		yes
15.1		Dangerous substances with restrictions (REACH, Annex XVII): change in the listing (table)	yes
15.1	List of substances subject to authorisation (REACH, Annex XIV)/SVHC - candidate list: Not listed.		yes
15.1	VOC content: 100 % , 877 g/l	VOC content: 100 %	yes
15.1		VOC content: 877 g/l	yes
15.1		National regulations(GB)	yes
15.1		List of substances subject to authorisation (GB REACH, Annex 14) / SVHC - candidate list: not listed	yes
15.1		Restrictions according to GB REACH, Annex 17	yes
15.1		Dangerous substances with restrictions (GB REACH, Annex 17): change in the listing (table)	yes
15.1		National inventories: change in the listing (table)	yes

#### Abbreviations and acronyms

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Abbr.	Descriptions of used abbreviations
ADR	Accord relatif au transport international des marchandises dangereuses par route (Agreement concerning the International Carriage of Dangerous Goods by Road)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
DGR	Dangerous Goods Regulations (see IATA/DGR)
EC50	Effective Concentration 50 %. The EC50 corresponds to the concentration of a tested substance causing 50 % changes in response (e.g. on growth) during a specified time interval
EC No	The EC Inventory (EINECS, ELINCS and the NLP-list) is the source for the seven-digit EC number, an identifier of substances commercially available within the EU (European Union)
ED	Endocrine disruptor
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
GB REACH	The REACH etc. (Amendment etc.) (EU Exit) Regulations 2019, SI 2019/758 (as amended)
GHS	"Globally Harmonized System of Classification and Labelling of Chemicals" developed by the United Nations
IATA	International Air Transport Association
IATA/DGR	Dangerous Goods Regulations (DGR) for the air transport (IATA)
ICAO	International Civil Aviation Organization
IMDG	International Maritime Dangerous Goods Code
LC50	Lethal Concentration 50%: the LC50 corresponds to the concentration of a tested substance causing 50 % lethality during a specified time interval
LD50	Lethal Dose 50 %: the LD50 corresponds to the dose of a tested substance causing 50 % lethality during a specified time interval
NLP	No-Longer Polymer
PBT	Persistent, Bioaccumulative and Toxic
PNEC	Predicted No-Effect Concentration
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

Agreement concerning the International Carriage of Dangerous Goods by Road (ADR). Regulations concerning the International Carriage of Dangerous Goods by Rail (RID). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

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

Code	Text
H315	Causes skin irritation.

### Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.