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

Crotonsäure ≥99 %, for biochemistry

date of compilation: 2021-03-08 article number: 1HHN Version: 1.0 en

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

Product identifier 1.1

Identification of the substance **Crotonsäure** ≥99 %, for biochemistry

Article number 1HHN

Registration number (REACH) 01-2119981250-42-xxxx

EC number 203-533-9 CAS number 107-93-7

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

Relevant identified uses: Laboratory and analytical use

Laboratory chemical

Uses advised against: Do not use for products which come into contact

with foodstuffs. Do not use for private purposes

(household).

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 Website: www.carlroth.de

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

sheet:

e-mail (competent person): 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

Classification of the substance or mixture

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

Section	Hazard class	Cat- egory	Hazard class and category	Hazard statement
3.3	Serious eye damage/eye irritation	1	Eye Dam. 1	H318

For full text of abbreviations: see SECTION 16

2.2 **Label elements**

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

Signal word Danger

Pictograms

GHS05



Hazard statements

H318 Causes serious eye damage

Precautionary statements

Precautionary statements - prevention

P280 Wear protective gloves/eye protection

Precautionary statements - response

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact

lenses, if present and easy to do. Continue rinsing

Labelling of packages where the contents do not exceed 125 ml

Signal word: Danger

Symbol(s)



H318 Causes serious eye damage.

P280 Wear protective gloves/eye protection.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to

do. Continue rinsing.

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.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance Crotonic acid

Molecular formula $C_4H_6O_2$

Molar mass 86,09 g/_{mol}

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SECTION 4: First aid measures

4.1 Description of first aid measures



General notes

Take off contaminated clothing.

Following inhalation

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

Following skin contact

Rinse skin with water/shower. In all cases of doubt, or when symptoms persist, seek medical advice.

Following eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

Following ingestion

Rinse mouth. Call a doctor if you feel unwell.

4.2 Most important symptoms and effects, both acute and delayed

Risk of blindness, Risk of serious damage to eyes, Cough, Dyspnoea, Headache, Nausea, Vomiting

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, foam, alcohol resistant foam, dry extinguishing powder, ABC-powder

Unsuitable extinguishing media

water jet

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 (CO₂)

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.

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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. Do not breathe dust.

6.2 Environmental precautions

Keep away from drains, surface and ground water.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains. Take up mechanically.

Advice on how to clean up a spill

Take up mechanically. Control of dust.

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. Use extractor hood (laboratory). Avoid dust formation.

Measures to prevent fire as well as aerosol and dust generation



Keep away from sources of ignition - No smoking.

Removal of dust deposits.

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

Store in a dry place.

Incompatible substances or mixtures

Observe hints for combined storage.

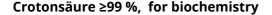
Consideration of other advice

Ventilation requirements

Use local and general ventilation.

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Specific designs for storage rooms or vessels

Recommended storage temperature: 15 - 25 °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)

Coun try	Name of agent	CAS No	Identifi- er	TWA [mg/ m³]	STEL [mg/ m³]	Ceil- ing-C [mg/ m³]	Nota- tion	Source
GB	dust		WEL	10			i	EH40/2005
GB	dust		WEL	4			r	EH40/2005

Notation

Ceiling value is a limit value above which exposure should not occur Inhalable fraction Ceiling-C

Respirable fraction

Short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified) STEL

Time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 TWA

hours time-weighted average (unless otherwise specified)

Environmental values

Relevant PNECs and other threshold levels

End- point	Threshold level	Organism	Environmental com- partment	Exposure time
PNEC	31 ^{µg} / _I	aquatic organisms	freshwater	short-term (single instance)
PNEC	3,1 ^{µg} / _l	aquatic organisms	marine water	short-term (single instance)
PNEC	5 ^{mg} / _l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	0,2 ^{mg} / _{kg}	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	0,02 ^{mg} / _{kg}	aquatic organisms	marine sediment	short-term (single instance)
PNEC	0,029 ^{mg} / _{kg}	terrestrial organisms	soil	short-term (single instance)

8.2 **Exposure controls**

Individual protection measures (personal protective equipment)

Eye/face protection



Use safety goggle with side protection.

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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 recommended.

Respiratory protection





Respiratory protection necessary at: Dust formation. Particulate filter device (EN 143). P1 (filters at least 80 % of airborne particles, colour code: White).

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 solid

Form powder, crystalline

Colour white
Odour stinging

Melting point/freezing point 71,5 – 71,7 °C (ECHA)

Boiling point or initial boiling point and boiling 185 °C at 1.013 hPa (ECHA)

range

Flammability this material is combustible, but will not ignite

readily

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Lower and upper explosion limit not determined

Flash point 88 °C at 1.013 hPa (ECHA)

Auto-ignition temperature >400 °C (ECHA)

Decomposition temperature not relevant

pH (value) \sim 3 (in aqueous solution: 10 9 /₁, 20 $^{\circ}$ C)

Kinematic viscosity not relevant

Solubility(ies)

Water solubility 94 ^g/_l at 25 °C (ECHA)

Partition coefficient

Partition coefficient n-octanol/water (log value): 0,85 (25 °C) (ECHA)

Vapour pressure 0,23 hPa at 20 °C

Density $1,018 \, \mathrm{g/_{cm^3}}$ at 15 °C

Bulk density $\sim 543 \, {}^{9}/_{cm^3}$

Particle characteristics No data available.

Other safety parameters

Oxidising properties none

9.2 Other information

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

Other safety characteristics: There is no additional information.

SECTION 10: Stability and reactivity

10.1 Reactivity

The product in the delivered form is not dust explosion capable; the enrichment of fine dust however leads to the danger of dust explosion.

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, Peroxides, Strong alkali

10.4 Conditions to avoid

Direct light irradiation. Keep away from heat.

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There is no additional information.

10.6 Hazardous decomposition products

Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008

Classification according to GHS (1272/2008/EC, CLP)

Acute toxicity

Acuto toxicity

Shall not be classified as acutely toxic.

Acute toxicity					
Exposure route	Endpoint	Value	Species	Method	Source
oral	LD50	2.610 ^{mg} / _{kg}	rat		ECHA
dermal	LD50	>2.000 ^{mg} / _{kg}	rat		ECHA

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye damage.

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

Causes serious eye damage, risk of blindness

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If inhaled

Data are not available.

• If on skin

Frequently or prolonged contact with skin may cause dermal irritation

Other information

Cough, Dyspnoea, Headache, Nausea, Vomiting Substance not yet fully tested

11.2 Endocrine disrupting properties

Not listed.

11.3 Information on other hazards

There is no additional information.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

Aquatic toxicity (acute)					
Endpoint	Value	Species	Exposure time		
LC50	31 ^{mg} / _l	fish	96 h		
EC50	150 ^{mg} / _l	aquatic invertebrates	48 h		

Biodegradation

The substance is readily biodegradable. The relevant substances of the mixture are readily biodegradable.

12.2 Process of degradability

Theoretical Oxygen Demand: 1,673 $^{\rm mg}/_{\rm mg}$ Theoretical Carbon Dioxide: 2,045 $^{\rm mg}/_{\rm mg}$

Process of degradability

Process	Degradation rate	Time
oxygen depletion	10 %	1 d

12.3 Bioaccumulative potential

Does not significantly accumulate in organisms.

12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

Data are not available.

12.6 Endocrine disrupting properties

Not listed.

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Data are not available.

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

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. Waste catalogue ordinance (Germany).

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	or ID	number

ADR/RID/ADN	UN 2823
IMDG-Code	UN 2823
ICAO-TI	UN 2823

14.2 UN proper shipping name

ADR/RID/ADN	CROTONIC ACID, SOLID
IMDG-Code	CROTONIC ACID, SOLID
ICAO-TI	Crotonic acid, solid

14.3 Transport hazard class(es)

ADR/RID/ADN	8
IMDG-Code	8
ICAO-TI	8

14.4 Packing group

ADR/RID/ADN	III
IMDG-Code	III
ICAO-TI	III

14.5 Environmental hazards non-environmentally hazardous acc. to the dan-

gerous goods regulations

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

14.7 Maritime transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN) - Additional information

Classification code C4
Danger label(s) 8



Excepted quantities (EQ)

Limited quantities (LQ)

Transport category (TC)

Tunnel restriction code (TRC)

Hazard identification No

Emergency Action Code

2X

International Maritime Dangerous Goods Code (IMDG) - Additional information

Marine pollutant Danger label(s) 8



Excepted quantities (EQ) E1
Limited quantities (LQ) 5 kg
EmS F-A, S-B
Stowage category A

Segregation group 1 - Acids

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Danger label(s) 8



Excepted quantities (EQ) E1
Limited quantities (LQ) 5 kg

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SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture Relevant provisions of the European Union (EU)

Restrictions according to REACH, Annex XVII

not listed

Not listed.

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

Seveso Directive

2012/	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 (2004/42/EC)

VOC content	100 % 1.018 ^g / _I
	·

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

VOC content	100 %
VOC content	1.018 ^g / _l

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

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

not listed

Water Framework Directive (WFD)

not listed

Regulation 98/2013/EU on the marketing and use of explosives precursors

Regulation 111/2005/EC laying down rules for the monitoring of trade between the Community and third countries in drug precursors

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

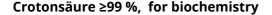
not listed

Regulation 649/2012/EU concerning the export and import of hazardous chemicals (PIC)

not listed

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National inventories

Country	Inventory	Status
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
NZ	NZIoC	substance is listed
TW	TCSI	substance is listed

Legend

CSCL-ENCS
ECSI EC Substance Inventory (EINECS, ELINCS, NLP)
IECSC Inventory of Existing Chemical Substances Produced or Imported in China KECI Korea Existing Chemicals Inventory
NZIOC New Zealand Inventory of Chemicals
REACH Reg. REACH registered substances
TCSI Taiwan Chemical Substance Inventory

15.2 Chemical Safety Assessment

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

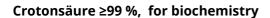
SECTION 16: Other information

Abbreviations and acronyms

Abbr.	Descriptions of used abbreviations
ADN	Accord européen relatif au transport international des marchandises dangereuses par voies de naviga- tion intérieures (European Agreement concerning the International Carriage of Dangerous Goods by In- land Waterways)
ADR	Accord européen relatif au transport international des marchandises dangereuses par route (European Agreement concerning the International Carriage of Dangerous Goods by Road)
ADR/RID/ADN	European Agreements concerning the International Carriage of Dangerous Goods by Road/Rail/Inland Waterways (ADR/RID/ADN)
CAS	Chemical Abstracts Service (service that maintains the most comprehensive list of chemical substances)
Ceiling-C	Ceiling value
CLP	Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures
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)
EH40/2005	EH40/2005 Workplace exposure limits (http://www.nationalarchives.gov.uk/doc/open-government-li- cence/)
EINECS	European Inventory of Existing Commercial Chemical Substances
ELINCS	European List of Notified Chemical Substances
EmS	Emergency Schedule

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Abbr.	Descriptions of used abbreviations
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
ICAO-TI	Technical instructions for the safe transport of dangerous goods by air
IMDG	International Maritime Dangerous Goods Code
IMDG-Code	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)
STEL	Short-term exposure limit
SVHC	Substance of Very High Concern
TWA	Time-weighted average
VOC	Volatile Organic Compounds
vPvB	Very Persistent and very Bioaccumulative
WEL	Workplace exposure limit

Key literature references and sources for data

Regulation (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures. Regulation (EC) No. 1907/2006 (REACH), amended by 2020/878/EU.

Transport of dangerous goods by road, rail and inland waterway (ADR/RID/ADN). 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 chapter 2 and 3)

Code	Text
H318	Causes serious eye damage.

Disclaimer

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

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