

Chemical Safety Data Sheet MSDS / SDS

Crotonic acid

Revision Date:2024-12-21 Revision Number:1

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

Product identifier

Product name : Crotonic acid
CBnumber : CB9145403
CAS : 3724-65-0
EINECS Number : 223-077-4
Synonyms : CROTONIC ACID,2-Butenoic acid

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 4, Oral
Acute toxicity - Category 4, Dermal
Skin corrosion, Sub-category 1C
Serious eye damage, Category 1

Label elements**Pictogram(s)**

☐

Signal word : Danger

Hazard statement(s)

H302 Harmful if swallowed
H312 Harmful in contact with skin
H314 Causes severe skin burns and eye damage

Precautionary statement(s)**Prevention**

P264 Wash ... thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P317 Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

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

P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Storage

P405 Store locked up.

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name	: Crotonic acid
Synonyms	: CROTONIC ACID,2-Butenoic acid
CAS	: 3724-65-0
EC number	: 223-077-4
MF	: C ₄ H ₆ O ₂
MW	: 86.09

SECTION 4: First aid measures

Description of first aid measures

If inhaled

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse skin with plenty of water or shower. Refer for medical attention .

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Do NOT induce vomiting. Rest. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: TOXIC; inhalation, ingestion or skin contact with material may cause severe injury or death. Contact with molten substance may cause severe burns to skin and eyes. Avoid any skin contact. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

Indication of any immediate medical attention and special treatment needed

For immediate first aid - Ensure that adequate decontamination has been carried out. If victim is not breathing, start artificial respiration, preferably with a demand valve resuscitator, bag-valve-mask, device or pocket mask as trained. Perform CPR if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep victim quiet and maintain normal body temperature. Obtain medical attention. Organic acids and related compounds

SECTION 5: Firefighting measures

Extinguishing media

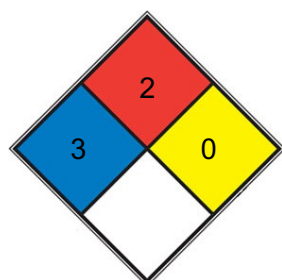
If material on fire or involved in fire: Use water in flooding quantities as fog. Solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. Use "alcohol" foam, dry chemical or carbon dioxide.

Specific Hazards Arising from the Chemical

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

NFPA 704

■	HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen , sulfuric acid , calcium hypochlorite , hexafluorosilicic acid)
<hr/>			
■	FIRE	2	Must be moderately heated or exposed to relatively high ambient temperature before ignition can occur and multiple finely divided suspended solids that do not require heating before ignition can occur. Flash point between 37.8 and 93.3 °C (100 and 200 °F). (e.g. diesel fuel, sulfur)
<hr/>			
■	REACT	0	Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, N2)
<hr/>			
□	SPEC.		
□	HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Consult an expert! Personal protection: complete protective clothing including self-contained breathing apparatus. Let solidify. Sweep spilled substance into covered containers. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from food and feedstuffs, bases, oxidants and reducing agents. Dry. Keep in the dark.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

Biological limit values

no data available

Exposure controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flammable resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Physical state	Crotonic acid is a white crystalline solid. Shipped as either a solid or liquid. Soluble in water and less dense than water. Corrosive to metals and tissue.
Colour	MONOCLINIC NEEDLES OR PRISMS (FROM WATER OR PETROLEUM ETHER)
Odour	no data available
Melting point/freezing point	73°C
Boiling point or initial boiling point and boiling range	181°C
Flammability	Combustible.
Lower and upper explosion limit/flammability limit	no data available
Flash point	88°C
Auto-ignition temperature	745 DEG F (396 DEG C)
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	no data available
Solubility	In water: soluble
Partition coefficient n-octanol/water	Log Kow = 0.72 /isomer not specified/
Vapour pressure	0.19 mm Hg (20 °C)
Density and/or relative density	1.027
Relative vapour density	2.97 (vs air)
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

The substance may polymerize under the influence of UV light or moisture. The solution in water is a weak acid. Reacts violently with bases, oxidants and reducing agents. This generates fire and explosion hazard.

Chemical stability

no data available

Possibility of hazardous reactions

MODERATE, WHEN EXPOSED TO HEAT OR FLAME CROTONIC ACID is a carboxylic acid. Carboxylic acids donate hydrogen ions if a base is present to accept them. They react in this way with all bases, both organic (for example, the amines) and inorganic. Their reactions with bases, called "neutralizations", are accompanied by the evolution of substantial amounts of heat. Neutralization between an acid and a base produces water plus a salt. Carboxylic acids with six or fewer carbon atoms are freely or moderately soluble in water; those with more than six carbons are slightly soluble in water. Soluble carboxylic acids dissociate to an extent in water to yield hydrogen ions. The pH of solutions of carboxylic acids is therefore less than 7.0. Many insoluble carboxylic acids react rapidly with aqueous solutions containing a chemical base and dissolve as the neutralization generates a soluble salt. Carboxylic acids in aqueous solution and liquid or molten carboxylic acids can react with active metals to form gaseous hydrogen and a metal salt. Such reactions occur in principle for solid carboxylic acids as well, but are slow if the solid acid remains dry. Even "insoluble" carboxylic acids may absorb enough water from the air and dissolve sufficiently in it to corrode or dissolve iron, steel, and aluminum parts and containers. Carboxylic acids, like other acids, react with cyanide salts to generate gaseous hydrogen cyanide. The reaction is slower for dry, solid carboxylic acids. Insoluble carboxylic acids react with solutions of cyanides to cause the release of gaseous hydrogen cyanide. Flammable and/or toxic gases and heat are generated by the reaction of carboxylic acids with diazo compounds, dithiocarbamates, isocyanates, mercaptans, nitrides, and sulfides. Carboxylic acids, especially in aqueous solution, also react with sulfites, nitrites, thiosulfates (to give H₂S and SO₃), dithionites (SO₂), to generate flammable and/or toxic gases and heat. Their reaction with carbonates and bicarbonates generates a harmless gas (carbon dioxide) but still heat. Like other organic compounds, carboxylic acids can be oxidized by strong oxidizing agents and reduced by strong reducing agents. These reactions generate heat. A wide variety of products is possible. Like other acids, carboxylic acids may initiate polymerization reactions; like other acids, they often catalyze (increase the rate of) chemical reactions.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

Thermal decomposition products include carbon dioxide and carbon monoxide. Organic acids and related compounds

SECTION 11: Toxicological information

Acute toxicity

- Oral: no data available

- Inhalation: no data available
- Dermal: no data available

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: no data available

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

Crotonic acid (mixture) was identified as being amenable to anaerobic biodegradation(1). Anaerobic bacteria isolated from mesophilic digester sludge acclimatized with 4-chlorobutyrate tentatively classified in the genus Clostridium, degraded crotonate to butyrate, acetate, and hydrogen(2). Ilyobacter polytropus anaerobically degraded crotonate to butyrate and acetate(2). Crotonate was degraded by an anaerobic bacterium to butyrate and acetate(3). After a lag period of 2 days, crotonic acid (isomer not specified) was metabolized, at a rate of 200 mg/l day, by anaerobic bacteria acclimated to acetate culture(4). Crotonic acid (isomer not specified) reached 44% of its theoretical BOD in 5 days using a sewage inoculum(5).

Bioaccumulative potential

An estimated BCF value of 2.1 was calculated for crotonic acid(SRC), using a measured log Kow of 0.72(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of crotonic acid is estimated as approximately 59(SRC), using a measured log Kow of 0.72(1) and a regression-derived equation(2,SRC). According to a classification scheme(3), this estimated Koc value suggests that crotonic acid is expected to have high mobility in soil(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN2823 (For reference only, please check.)

IMDG: UN2823 (For reference only, please check.)

IATA: UN2823 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: CROTONIC ACID, SOLID (For reference only, please check.)

IMDG: CROTONIC ACID, SOLID (For reference only, please check.)

IATA: CROTONIC ACID, SOLID (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.)

IMDG: 8 (For reference only, please check.)

IATA: 8 (For reference only, please check.)

Packing group, if applicable

ADR/RID: III (For reference only, please check.)

IMDG: III (For reference only, please check.)

IATA: III (For reference only, please check.)

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pagelD=0&request_locale=en

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

Disclaimer:

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