

Chemical Safety Data Sheet MSDS / SDS

Crotonaldehyde

Revision Date:2024-07-27 Revision Number:1

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

Product identifier

Product name : Crotonaldehyde
CBnumber : CB3733701
CAS : 123-73-9
EINECS Number : 204-647-1
Synonyms : Crotonaldehyde,2-Butenal

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

Flammable liquids, Category 2
Acute toxicity - Category 3, Oral
Acute toxicity - Category 3, Dermal
Skin irritation, Category 2
Serious eye damage, Category 1
Acute toxicity - Category 2, Inhalation
Specific target organ toxicity – single exposure, Category 3
Germ cell mutagenicity, Category 2
Specific target organ toxicity – repeated exposure, Category 2
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Label elements

Pictogram(s)

□□□□

Signal word

Danger

Hazard statement(s)

H225 Highly Flammable liquid and vapour
H315 Causes skin irritation
H318 Causes serious eye damage
H330 Fatal if inhaled
H335 May cause respiratory irritation
H341 Suspected of causing genetic defects
H373 May cause damage to organs through prolonged or repeated exposure
H400 Very toxic to aquatic life

Precautionary statement(s)

P201 Obtain special instructions before use.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P370+P378 In case of fire: Use ... for extinction.

Prevention

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof [electrical/ventilating/lighting/...] equipment.
P242 Use non-sparking tools.
P243 Take action to prevent static discharges.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P203 Obtain, read and follow all safety instructions before use.
P273 Avoid release to the environment.

Response

P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse affected areas with water [or shower].
P370+P378 In case of fire: Use ... to extinguish.
P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue

rinsing.

P317 Get medical help.

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

P320 Specific treatment is urgent (see ... on this label).

P319 Get medical help if you feel unwell.

P318 IF exposed or concerned, get medical advice.

P391 Collect spillage.

Storage

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

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 | : Crotonaldehyde |
| Synonyms | : Crotonaldehyde,2-Butenal |
| CAS | : 123-73-9 |
| EC number | : 204-647-1 |
| MF | : C ₄ H ₆ O |
| MW | : 70.09 |

SECTION 4: First aid measures

Description of first aid measures

If inhaled

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

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. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

Although slightly less toxic, crotonaldehyde is similar chemically and toxicologically to acrolein, which is rated as extremely toxic. Toxic

concentrations for human inhalation have been reported at 12 mg/m³/10 minutes. Irritant dose to human eye is 45 ppm. As with acrolein, vapor exposures cause severe and painful eye irritation, damage to cornea, lacrimation (tearing), irritation of nasal membranes, pulmonary edema (filling of lungs with fluid) and gastrointestinal distress when ingested. (EPA, 1998)

This compound is an extreme eye, respiratory, and skin irritant and can cause corneal damage. A 15 minute exposure at 4.1 ppm is highly irritating to the nose and upper respiratory tract and causes tearing. Brief exposure at 45 ppm proved very disagreeable with prominent eye irritation. (EPA, 1998)

Indication of any immediate medical attention and special treatment needed

Prehospital Management. Victims exposed only to crotonaldehyde vapor do not pose contamination risks to rescuers. Victims whose clothing or skin is contaminated with liquid crotonaldehyde can secondarily contaminate response personnel by direct contact or by off-gassing vapor. Crotonaldehyde is a direct irritant to mucous membranes, skin, eyes, and the respiratory system. Acute inhalation exposure may lead to respiratory distress and noncardiogenic pulmonary edema. There is no antidote for crotonaldehyde. Treatment consists of respiratory and cardiovascular support.

SECTION 5: Firefighting measures

Extinguishing media

Evacuation: If fire becomes uncontrollable or container is exposed to direct flame-consider evacuation of one-third (1/3) mile radius.

Crotonaldehyde, stabilized

Specific Hazards Arising from the Chemical

Vapors form explosive mixtures in air or in sewers. Hazardous peroxides and acids emitted when heated to decomposition. Avoid nitric acid.

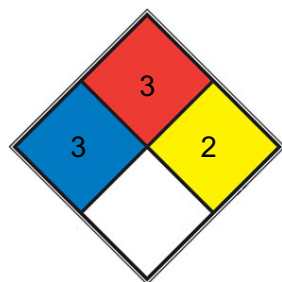
Unstable, avoid oxygen, heat, elevated pressures. Hazardous polymerization may occur. Avoid contact with alkaline materials such as caustic ammonia or amines, or at elevated temperatures. (EPA, 1998)

Flammable/combustible material; may be ignited by heat, sparks or flames. Vapor may travel to a source of ignition and flash back. Container may explode in heat of fire. Vapor explosion and poison hazard indoors, outdoors or in sewers. Runoff to sewer may create fire or explosion hazard. Readily converted by oxygen to hazardous peroxides and acids and is incompatible with caustics, ammonia, organic amines, mineral acids, and strong oxidizers. Readily resinifies to dimer when pure and slowly oxidizes to crotonic acid. Altered by light and air. Hazardous polymerization may occur. Polymerization may take place at high temperatures. (EPA, 1998)

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)

Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature

- FIRE 3 conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))
-
- REACT 2 Undergoes violent chemical change at elevated temperatures and pressures, reacts violently with water, or may form explosive mixtures with water (e.g. white phosphorus, [potassium](#), [sodium](#))
-
- 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

Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Ventilation. Remove all ignition sources. Do NOT absorb in saw-dust or other combustible absorbents. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in sealable containers as far as possible. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Environmental considerations land spill: Dig a pit, pond, lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner. / Dike surface flow using soil, sand bags, foamed polyurethane, or foamed concrete. Absorb bulk liquid with fly ash or cement powder. Apply appropriate foam to diminish vapor and fire hazard. Add sodium bisulfite (NaHSO₃). Crotonaldehyde, stabilized

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

Fireproof. Separated from food and feedstuffs. See Chemical Dangers. Cool. Keep in the dark. Well closed. Store only if stabilized. Store in cool place with containers tightly sealed & away from sources of ignition or heat.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

| | | | | |
|--------------------|--|-------------------------|---------------------------------|-------------------------|
| Component | (E)-crotonaldehyde | | | |
| CAS No. | 123-73-9 | | | |
| | Limit value - Eight hours | | Limit value - Short term | |
| | ppm | mg/m³ | ppm | mg/m³ |
| Austria | 0,34 | 1 | 1,36 | 4 |
| Denmark | 2 | 6 | 4 | 12 |
| Finland | 0,1 | 0,29 | 0,3 (1) | 0,87 (1) |
| France | 2 | 6 | ? | ? |
| Ireland | 2 | 6 | 6 (1) | 18 (1) |
| Spain | ? | ? | 0,3 | 0,87 |
| Switzerland | 0,34 | 1 | ? | ? |
| USA - NIOSH | 2 | 6 | ? | ? |
| USA - OSHA | 2 | 6 | ? | ? |
| | Remarks | | | |
| Austria | TRK value (based on technical feasibility) | | | |
| Finland | (1) 15 minutes average value | | | |
| Ireland | (1) 15 minutes reference period | | | |
| Spain | skin | | | |

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 | Liquid |
| Colour | Clear |
| Odour | Pungent, suffocating odor |

| | |
|--|---|
| Melting point/freezing point | -74°C |
| Boiling point or initial boiling point and boiling range | 101-103°C |
| Flammability | Class IB Flammable Liquid: Fl.P. below 73°F and BP at or above 100°F. |
| Lower and upper explosion limit/flammability limit | 19.5% |
| Flash point | 13°C |
| Auto-ignition temperature | 450° F (USCG, 1999) |
| Decomposition temperature | no data available |
| pH | no data available |
| Kinematic viscosity | no data available |
| Solubility | water: soluble 425.4g/L at 20°C |
| Partition coefficient n-octanol/water | log Kow = 0.60 (est) |
| Vapour pressure | 32 mm Hg (20 °C) |
| Density and/or relative density | 0.858 |
| Relative vapour density | 2.41 (vs air) |
| Particle characteristics | no data available |

SECTION 10: Stability and reactivity

Reactivity

The substance can presumably form explosive peroxides. The substance may polymerize. This generates fire or explosion hazard. The substance is a strong reducing agent. It reacts violently with oxidants and many other substances. This generates fire and explosion hazard. Attacks plastics and many other substances.

Chemical stability

May deteriorate in normal storage & cause hazard.

Possibility of hazardous reactions

Fire hazard ... when exposed to heat or flame; can react with oxidizing materials. The vapour is heavier than air and may travel along the ground; distant ignition possible. (E)-CROTONALDEHYDE is an aldehyde. It can react violently with strong oxidizing reagents, e.g., reaction with conc. nitric acid leads to instantaneous ignition [Andrussow, L., Chim. Ind. (Paris), 1961, 86, p. 542]. In contact with strong acids or bases it will undergo an exothermic condensation reaction. Reaction with 1,3-butadiene is particularly violent [Greenlee, K. W., Chem. Eng. News, 1948, 26, p. 1985]. Crotonaldehyde may rapidly polymerize with ethyl acetoacetate (Soriano, D.S. et al. 1988. Journal of Chemical Education 65:637.).

Conditions to avoid

no data available

Incompatible materials

The Diels-Adler reaction between ... /1,3-butadiene & crotonaldehyde/ under pressure is a logical approach to the prepn of a number of cyclic aldehydes, alcohols, & hydrocarbons. A destructive explosion, including a secondary gas explosion, occurred in carrying out this reaction.

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 206 mg/kg
- Inhalation: LC50 Rat inhalation 200 mg/cu m/ 2hr
- 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

CLASSIFICATION: C; possible human carcinogen. BASIS FOR CLASSIFICATION: Based on no human data and an increased incidence of hepatocellular carcinomas and hepatic neoplastic nodules (combined) in male F344 rats. The possible carcinogenicity of crotonaldehyde is supported by genotoxic activity and the expected reactivity of croton oil and aldehyde. Crotonaldehyde is also a suspected metabolite of N-nitrosopyrrolidine, a probable human carcinogen. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: Limited.

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: LC50; Species: *Lepomis macrochirus* (Bluegill sunfish); Conditions: static bioassay in fresh water at 23 deg C with mild aeration

applied after 24 hr; Concentration: 3.5 ppm for 96 hr (85% aqueous)

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater, static;

Concentration: 3900 ug/L for 24 hr; Effect: behavior equilibrium

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

Crotonaldehyde (isomer not reported) was observed to have a 5-day BODT of 37% using the AFNOR T.90 test protocol(1). (E)-

Crotonaldehyde has been found to be degradable via anaerobic (methane fermentation) biotechnology(2,3).

Bioaccumulative potential

An estimated BCF value of 0.74 was calculated for (E)-crotonaldehyde(SRC), using an experimental water solubility of 150,000 mg/L at 20 deg C(1), and a recommended regression-derived equation(2). According to a recommended classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms will not be an important fate process(SRC).

Mobility in soil

The Koc of (E)-crotonaldehyde is estimated to be approximately 6.2(SRC), using an experimental water solubility of 150,000 mg/L at 20 deg C(1) and a regression-derived equation(2,SRC). According to a recommended classification scheme(3), this estimated Koc value suggests that (E)-crotonaldehyde has very 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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (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: Yes

IMDG: Yes

IATA: Yes

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

Not 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/>

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