

Product name Crotonaldehyde  
MSDS number 80560  
Revision Number 2.00

EUIE/EN

Revision Date Feb.02.2007  
Issuing date Feb.02.2007

## 1. Identification of the substance/preparation and the company/undertaking

Product name  
**Crotonaldehyde**

**Manufacturer, importer, supplier**  
Celanese Chemicals Europe GmbH  
Frankfurter Straße 111  
D-61476 Kronberg/Ts.

**Product Information**  
Product Stewardship FAX +49 (0) 208 693 2053

**Emergency telephone number**  
+49 (0) 69-305 6418

**End use:**  
Chemical intermediate (including monomers)

## 2. Composition/information on ingredients

**Chemical characterization** 2-Butenal, 3-Methylacroleine (also CAS-No. 123-73-9, EINECS-No. 204-647-1).

Components	CAS-No	EC-No.	Classification	Percent %
Crotonaldehyde	4170-30-3	224-030-0	F;R11 Muta. Cat.3;R68 N;R50 T+;R26 T;R24/25 Xi;R37/38-41 Xn;R48/22	> 99.0

## 3. Hazards identification

**Indication of danger** Highly flammable  
Dangerous for the environment  
Very Toxic

**R-phrases(s)**  
R11 - Highly flammable.  
R26 - Very toxic by inhalation.  
R41 - Risk of serious damage to eyes.  
R50 - Very toxic to aquatic organisms.  
R68 - Possible risks of irreversible effects.

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R24/25 - Toxic in contact with skin and if swallowed.  
 R37/38 - Irritating to respiratory system and skin.  
 R48/22 - Harmful: danger of serious damage to health by prolonged exposure if swallowed.

**Statements of hazard** In addition to the EC classification based on Celanese data this product should also be regarded as:  
 corrosive  
 May cause sensitization by skin contact

**4. First aid measures**

**General Information** Remove contaminated, soaked clothing immediately and dispose of safely.  
**Inhalation** Keep at rest. Aerate with fresh air. If symptoms persist, call a physician.  
**Skin** Wash off immediately with soap and plenty of water. If symptoms persist, call a physician.  
**Eyes** Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Call a physician immediately.  
**Ingestion** Call a physician immediately. Do not induce vomiting without medical advice.

**Notes to physician**

**Main symptoms** Shortness of breath.  
**Special hazard** Lung oedema.  
**Treatment** Treat symptomatically. In case of lung irritation first treatment with dexametason aerosol (spray).

**5. Fire-fighting measures**

**Suitable extinguishing media**  
 alcohol-resistant foam. Dry chemical. carbon dioxide (CO2).

**Extinguishing media which must not be used for safety reasons**  
 Do not use a solid water stream as it may scatter and spread fire.

**Special exposure hazards arising from the substance or preparation itself, its combustion products, or released gases**

Under conditions giving incomplete combustion, hazardous gases produced may consist of carbon monoxide carbon dioxide (CO2)  
 Combustion gases of organic materials must in principle be graded as inhalation poisons vapors are heavier than air and may spread along floors

**Special protective equipment for fire-fighters**  
 self-contained breathing apparatus (EN 133).

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**Environmental precautions**

Dike and collect water used to fight fire.

**Other Information**

Cool containers / tanks with water spray.

**6. Accidental release measures****Personal precautions**

Provide adequate ventilation. Avoid contact with the skin and the eyes. Keep away from heat and sources of ignition.

**Environmental precautions**

Prevent further leakage or spillage. Do not discharge into the drains/surface waters/groundwater.

**Methods for cleaning Up**

Soak up with inert absorbent material. Do not use rags, paper towels or combustible materials to clean up a spill, because spontaneous combustion can occur. Keep in suitable, closed containers for disposal. Dispose of in accordance with local regulations.

**7. Handling and storage****Handling****Advice on safe handling**

Provide sufficient air exchange and/or exhaust in work rooms. Refill and handle product only in closed system.

**Protection - fire and explosion:**

Keep away from sources of ignition - No smoking. Take necessary action to avoid static electricity discharge. Ground and bond containers when transferring material. In case of fire, emergency cooling with water spray should be available. Vapours are heavier than air and may spread along floors.

**Temperature class**

T4

**Storage****Technical measures/Storage conditions**

Keep tightly closed in a dry, cool and well-ventilated place. Handle and open container with care. Store under nitrogen.

**Incompatible products**

strong acids. oxidizing agents. strong bases.

**German storage class**

3A: Flammable liquids.

**8. Exposure controls / personal protection****National occupational exposure limits**

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No exposure limits established.

**Engineering measures**                      General or dilution ventilation is frequently insufficient as the sole means of controlling employee exposure. Local ventilation is usually preferred. Explosion-proof equipment (for example fans, switches, and grounded ducts) should be used in mechanical ventilation systems.

**Personal protective equipment**

**General advice**                              Avoid contact with skin and eyes. Do not breathe vapors or spray mist. Use only in an area equipped with a safety shower. Hold eye wash fountain available.

**Hygiene measures**                         When using, do not eat, drink or smoke. Take off all contaminated clothing immediately. Wash hands before breaks and immediately after handling the product.

**Respiratory protection**                 respirator with A filter. Full mask with above mentioned filter according to producers using requirements or self-contained breathing apparatus. Equipment should conform to EN 136 or EN 140 and EN 143.

**Eye protection**                             tightly fitting safety goggles. In addition to goggles, wear a face shield if there is a reasonable chance for splash to the face. Equipment should conform to EN 166.

**skin protection**                             impervious clothing

**Hand protection**  
**Chemicals resistant gloves**

<b>Suitable material</b>	butyl-rubber
<b>Type</b>	Butylplus (Company COMASEC) or comparable article; or refer to glove manufacturer's recommendation
<b>Evaluation</b>	according to EN 374: level 4
<b>Material thickness</b>	approx 0.3 mm
<b>Break through time</b>	approx 120 min

**9. Physical and chemical properties**

**Appearance**

<b>Form</b>	liquid
<b>Colour</b>	yellowish
<b>Odor</b>	pungent

<b>Molecular Weight</b>	70.09
<b>Flash point</b>	13°C
<b>Method</b>	closed cup

<b>Ignition temperature</b>	155°C
<b>Method</b>	DIN 51794

<b>Lower explosion limit</b>	2.1 Vol. %
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<b>Upper explosion limit</b>	15.5 Vol. %
<b>Melting point/range</b>	-76.5°C
<b>Boiling point/range</b>	102°C @ 1013 hPa
<b>Density</b>	0.85 g/ml @ 20°C
<b>vapor pressure</b>	40 hPa @ 25°C
<b>vapor density</b>	2.41 (Air=1 @ 20 °C)
<b>Water solubility</b>	150 g/l @ 20°C
<b>Partition coefficient (n-octanol/water)</b>	0.60 (calculated)

## 10. Stability and reactivity

<b>Stability</b>	Stable under normal conditions of handling, use and transportation.
<b>Conditions to avoid</b>	Avoid any source of ignition. Avoid contact with heat, sparks, open flame, and static discharge.
<b>Materials to avoid</b>	Keep away from:., strong acids, oxygen, oxidizing agents, bases, amines.
<b>Thermal decomposition</b>	No decomposition if used as directed. If heated to thermal decomposition the following decomposition products may occur depending on the conditions. carbon oxides.
<b>Hazardous reactions</b>	May form explosive peroxides. Polymerization can occur. Polymerization is a highly exothermic reaction and may generate sufficient heat to cause thermal decomposition and/or rupture containers.

## 11. Toxicological information

<b>Crotonaldehyde</b>	
<b>Oral</b>	LD50: 174 - 300 mg/kg, rat
<b>Dermal</b>	LD50: 324 mg/kg, rabbit
<b>Inhalation</b>	LC50: 0.2 mg/l, rat, 2h
<b>Skin irritation</b>	corrosive
Species	rabbit
Method	Exposure time: 4 h occluded treatment
<b>Skin Sensitization</b>	moderate sensitizer
Species	Human experience
<b>Eye Irritation</b>	corrosive
Species	rabbit eye
<b>Carcinogenic effects</b>	Induced neoplastic lesions of the liver in 9 of 27 animals and precancerous altered liver foci in 23 of 27 animals
Species	rats
Study	oral (drinking water) lifetime study
	LOAEL: 0.6 mM

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<b>in vitro Mutagenicity</b>	Ames test - positive Induces DNA-protein cross-links Induces DNA adducts in primary rat liver, CHO and human cells
<b>in vivo Mutagenicity</b>	Induces sex-linked recessive mutations and chromosome translocations in the fruit fly by injection
<b>Reproductive toxicity</b>	Induces damage to mouse spermatogonial cells and aneuploidy by oral and IP treatment
<b>Repeated exposure</b>	90-day Damage of forestomach including necrosis at a dose of $\geq 10$ mg/kg/day
Routes of exposure	oral gavage
Species	rats NOAEL: 5 mg/kg/day
Species	mice NOAEL: 20 mg/kg/d

## 12. Ecological information

### Crotonaldehyde

<b>Toxicity to fish</b>	LC50: 3.5 mg/l (96h)
Species	Lepomis macrochirus (Bluegill sunfish)
Method	static conditions
Species	LC50: 0.96 mg/l (96h)
Method	Pimephales promelas (Fathead minnow) Flow-through
<b>Toxicity to daphnia</b>	EC50: 1.8 mg/l (48h)
Species	Daphnia magna
<b>Toxicity to algae</b>	EC50: 0.88 mg/l (48h)
Species	Selenastrum capricornutum (green algae)
<b>Biodegradation</b>	37 % (5d)
<b>Bioconcentration factor (BCF)</b>	-0.17

## 13. Disposal considerations

<b>Product information</b>	Disposal required in compliance with all waste management related state and local regulations. The choice of the appropriate method of disposal depends on the product composition by the time of disposal as well as the local statutes and possibilities for disposal.
<b>Uncleaned empty packaging</b>	Contaminated packaging should be emptied as far as possible and after appropriate cleansing may be taken for reuse.

## 14. Transport information

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## **14. Transport information**

### **ADR/RID**

UN/ID No. UN 1143  
Proper Shipping Name Crotonaldehyde  
Hazard Class 6.1  
Subsidiary Risk 3  
Packing group I  
Hazard Number 663

### **ADNR**

ADNR: Container and Tanker  
UN/ID No. UN 1143  
Proper Shipping Name Crotonaldehyde  
Hazard Class 6.1  
Subsidiary Risk 3  
Packing group I

ICAO/IATA forbidden

### **IMDG**

UN/ID No. UN 1143  
Proper Shipping Name Crotonaldehyde  
Hazard Class 6.1  
Subsidiary Risk 3  
Packing group I  
Marine pollutant Yes  
EmS Code F-E, S-D

## **15. Regulatory information**

### **Labelling in accordance with EC directives**

EC label

**Contains** Crotonaldehyde

**Symbol(s)** F - Highly flammable.  
T+ - Very toxic.  
N - Dangerous for the environment.

**R-phrases(s)**

R11 - Highly flammable.  
R26 - Very toxic by inhalation.  
R41 - Risk of serious damage to eyes.  
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R24/25 - Toxic in contact with skin and if swallowed.  
 R37/38 - Irritating to respiratory system and skin.  
 R48/22 - Harmful: danger of serious damage to health by prolonged exposure if swallowed.

**S-phrase(s)**

S26 - In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.  
 S28.2 - After contact with skin, wash immediately with plenty of soap and water.  
 S61 - Avoid release to the environment. Refer to special instructions/Safety data sheets.  
 S36/37/39 - Wear suitable protective clothing, gloves and eye/face protection.

**Directive 1996/82/EC**

Annex I, part 2:  
 No 1  
 No 7b  
 No 9i

**Water Hazard Class (WGK):**

**WGK Class** 3  
**WGK Reg-Nr.** 239  
**WGK Source** Classification according to VwVwS, Annex 1 or 2

Crotonaldehyde 4170-30-3

**Directive 76/769/EEC** Listed.

**Directive 98/24/EC** Listed.

**16. Other information**

**R-phrase(s)**

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**For further information, see:**

For more information, other material safety data sheets or technical data sheets please consult the Celanese homepage ([www.celanese.com](http://www.celanese.com)).

**Other Information:**

Observe national and local legal requirements.

Changes against the previous version are marked by \*\*\*



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**Sources of key data used to compile the datasheet**

Information contained in this safety data sheet is based on Celanese owned data and public sources deemed valid or acceptable. The absence of data elements required by ANSI or 2001/58/EC indicates, that no data meeting these requirements is available.

**Further information**

This information is based on our present state of knowledge. It shall describe our products regarding safety requirements and shall not be construed as a guarantee or statement of condition and/or quality