

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 05.02.2015

Version 5.1

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

### 1.1 Product identifier

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis
REACH Registration Number	A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	623-68-7

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

Identified uses	Chemical for synthesis For additional information on uses please refer to the Merck Chemicals portal ( <a href="http://www.merckgroup.com">www.merckgroup.com</a> ).
-----------------	---

### 1.3 Details of the supplier of the safety data sheet

Company	Merck KGaA * 64271 Darmstadt * Germany * Phone:+49 6151 72-0
Responsible Department	LS-QHC * e-mail: <a href="mailto:prodsafe@merckgroup.com">prodsafe@merckgroup.com</a>

### 1.4 Emergency telephone number

Please contact the regional company representation in your country.

## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification (REGULATION (EC) No 1272/2008)

Specific target organ toxicity - single exposure, Category 3, H335  
 Skin irritation, Category 2, H315  
 Serious eye damage, Category 1, H318  
 Acute aquatic toxicity, Category 1, H400

For the full text of the H-Statements mentioned in this Section, see Section 16.

#### Classification (67/548/EEC or 1999/45/EC)

Xi	Irritant	R41 - 37/38
N	Dangerous for the environment	R50

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 2.2 Label elements

#### Labelling (REGULATION (EC) No 1272/2008)

##### Hazard pictograms



SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 822002  
Product name Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

*Signal word*

Danger

*Hazard statements*

H315 Causes skin irritation.  
H318 Causes serious eye damage.  
H335 May cause respiratory irritation.  
H400 Very toxic to aquatic life.

*Precautionary statements*

Prevention

P273 Avoid release to the environment.  
P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P304 + P340 IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.  
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P313 Get medical advice/ attention.

**Reduced labelling (≤125 ml)**

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H318 Causes serious eye damage.

*Precautionary statements*

P280 Wear 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.  
P313 Get medical advice/ attention.

CAS-No. 623-68-7

**2.3 Other hazards**

None known.

---

**SECTION 3. Composition/information on ingredients**

**3.1 Substance**

Formula	$(\text{CH}_3\text{CH}=\text{CHCO})_2\text{O}$	$\text{C}_8\text{H}_{10}\text{O}_3$ (Hill)
EC-No.	210-807-1	
Molar mass	154,17 g/mol	

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis

## Hazardous components (REGULATION (EC) No 1272/2008)

*Chemical Name (Concentration)*

CAS-No.	Registration number	Classification
---------	---------------------	----------------

trans-crotonic anhydride ( $\geq 50\%$  -  $\leq 100\%$ )

78957-07-0 \*)

Skin irritation, Category 2, H315

Serious eye damage, Category 1, H318

Specific target organ toxicity - single exposure, Category 3, H335

Acute aquatic toxicity, Category 1, H400

cis-crotonic anhydride ( $\geq 5\%$  -  $< 10\%$ )

- \*)

Skin corrosion, Category 1B, H314

\*) A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

For the full text of the H-Statements mentioned in this Section, see Section 16.

## Hazardous components (1999/45/EC)

*Chemical Name (Concentration)*

CAS-No.	Classification
---------	----------------

trans-crotonic anhydride ( $\geq 50\%$  -  $\leq 100\%$ )

78957-07-0 Xi, Irritant; R37/38-41

N, Dangerous for the environment; R50

cis-crotonic anhydride ( $\geq 5\%$  -  $< 10\%$ )

- C, Corrosive; R34

For the full text of the R-phrases mentioned in this Section, see Section 16.

### 3.2 Mixture

Not applicable

## SECTION 4. First aid measures

### 4.1 Description of first aid measures

After inhalation: fresh air. Consult doctor if feeling unwell.

After skin contact: wash off with plenty of water. Remove contaminated clothing.

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist.

After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.

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

irritant effects, Headache

Risk of serious damage to eyes.

### 4.3 Indication of any immediate medical attention and special treatment needed

No information available.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

---

## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

powder, Carbon dioxide (CO<sub>2</sub>), Dry powder

*Unsuitable extinguishing media*

Water, Foam

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

Combustible material, Vapours are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air on intense heating.

### 5.3 Advice for firefighters

*Special protective equipment for firefighters*

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

*Further information*

Cool closed containers exposed to fire with water spray. Prevent fire extinguishing water from contaminating surface water or the ground water system.

---

## SECTION 6. Accidental release measures

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

Advice for non-emergency personnel: Avoid substance contact. Do not breathe vapours, aerosols. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

Advice for emergency responders: Protective equipment see section 8.

### 6.2 Environmental precautions

Do not empty into drains.

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

Cover drains. Collect, bind, and pump off spills.

Observe possible material restrictions (see sections 7 and 10).

Take up with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

Indications about waste treatment see section 13.

---

## SECTION 7. Handling and storage

### 7.1 Precautions for safe handling

*Advice on safe handling*

Observe label precautions.

*Hygiene measures*

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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

*Storage conditions*

Tightly closed.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 822002  
Product name Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

Recommended storage temperature see product label.

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated.

---

**SECTION 8. Exposure controls/personal protection**

**8.1 Control parameters**

**8.2 Exposure controls**

**Engineering measures**

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

See section 7.1.

**Individual protection measures**

Protective clothing needs to be selected specifically for the workplace, depending on concentrations and quantities of the hazardous substances handled. The chemical resistance of the protective equipment should be enquired at the respective supplier.

*Eye/face protection*

Tightly fitting safety goggles

*Hand protection*

full contact:

Glove material:	butyl-rubber
Glove thickness:	0,7 mm
Break through time:	> 480 min

splash contact:

Glove material:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 730 Camatril® -Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet(>,<)> supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

*Respiratory protection*

required when vapours/aerosols are generated.

**Environmental exposure controls**

Do not empty into drains.

---

**SECTION 9. Physical and chemical properties**

**9.1 Information on basic physical and chemical properties**

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 822002  
Product name Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

Form	liquid
Colour	yellow
Odour	stinging
Odour Threshold	No information available.
pH	No information available.
Melting point	-20 °C
Boiling point/boiling range	250 °C
Flash point	113 °C
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	No information available.
Upper explosion limit	No information available.
Vapour pressure	1 hPa at 25 °C
Relative vapour density	No information available.
Density	1,04 g/cm <sup>3</sup> at 20 °C
Relative density	No information available.
Water solubility	at 20 °C (decomposition)
Partition coefficient: n-octanol/water	log Pow: 0,96 (experimental) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	3 mPa.s at 20 °C
Explosive properties	No information available.
Oxidizing properties	No information available.

## 9.2 Other data

Ignition temperature	290 °C
----------------------	--------

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

---

**SECTION 10. Stability and reactivity**

**10.1 Reactivity**

hydrolyses  
Forms explosive mixtures with air on intense heating.

**10.2 Chemical stability**

The product is chemically stable under standard ambient conditions (room temperature) .

**10.3 Possibility of hazardous reactions**

Water, alkalines, Strong oxidizing agents

**10.4 Conditions to avoid**

Strong heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.  
Exposure to moisture.

**10.5 Incompatible materials**

no information available

**10.6 Hazardous decomposition products**

no information available

---

**SECTION 11. Toxicological information**

**11.1 Information on toxicological effects**

*Acute oral toxicity*

LD50 Rat: 2.061 mg/kg  
OECD Test Guideline 401

*Acute inhalation toxicity*

This information is not available.

*Acute dermal toxicity*

This information is not available.

*Skin irritation*

Rabbit  
Result: Irritations  
(External MSDS)  
Causes skin irritation.

*Eye irritation*

Rabbit  
Result: Irritations  
(External MSDS)  
Causes serious eye damage.

*Sensitisation*

This information is not available.

*Germ cell mutagenicity*

This information is not available.

*Carcinogenicity*

This information is not available.

*Reproductive toxicity*

This information is not available.

---

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

*Teratogenicity*

This information is not available.

*Specific target organ toxicity - single exposure*

May cause respiratory irritation.

*Specific target organ toxicity - repeated exposure*

This information is not available.

*Aspiration hazard*

This information is not available.

## 11.2 Further information

Decomposition of the substance with tissue moisture., After inhalation: Irritations of the mucous membranes, coughing, and dyspnoea., Possible damages:, Lung oedema, The substance has delayed effects., After skin contact: Irritations., In case of eye contact, Risk of serious damage to eyes., If swallowed, Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract., Systemic effects:, Headache

Other dangerous properties can not be excluded., Handle in accordance with good industrial hygiene and safety practice.

---

## SECTION 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

LC50 Danio rerio (zebra fish): 0,5 - 1 mg/l; 96 h (External MSDS)

*Toxicity to bacteria*

fermentation tube test EC0 Bacteria: > 2.500 mg/l(External MSDS)

### 12.2 Persistence and degradability

*Biodegradability*

> 95 %

OECD Test Guideline 302B

OECD Test Guideline 302B

Readily biodegradable.

### 12.3 Bioaccumulative potential

*Partition coefficient: n-octanol/water*

log Pow: 0,96

(experimental)

Bioaccumulation is not expected.

### 12.4 Mobility in soil

No information available.

### 12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted.

### 12.6 Other adverse effects

*Additional ecological information*

Discharge into the environment must be avoided.



SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

## SECTION 13. Disposal considerations

### *Waste treatment methods*

See [www.retrologistik.com](http://www.retrologistik.com) for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

---

## SECTION 14. Transport information

### Land transport (ADR/RID)

14.1 UN number	UN 3082
14.2 Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (CROTONIC ANHYDRIDE)
14.3 Class	9
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
Tunnel restriction code	E

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

### Inland waterway transport (ADN)

Not relevant

### Air transport (IATA)

14.1 UN number	UN 3082
14.2 Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (CROTONIC ANHYDRIDE)
14.3 Class	9
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	no

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

### Sea transport (IMDG)

14.1 UN number	UN 3082
14.2 Proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, LIQUID, N.O.S. (CROTONIC ANHYDRIDE)
14.3 Class	9
14.4 Packing group	III
14.5 Environmentally hazardous	yes
14.6 Special precautions for user	yes
EmS	F-A S-F

Packages smaller than or equal to 5 kg / L , not dangerous goods of Class 9

**14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code**  
Not relevant

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No.	822002
Product name	Crotonic anhydride (mixture of cis and trans isomers) for synthesis

---

**SECTION 15. Regulatory information**

**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

*EU regulations*

Major Accident Hazard	96/82/EC
Legislation	Dangerous for the environment
	9a
	Quantity 1: 100 t
	Quantity 2: 200 t

Occupational restrictions	Take note of Dir 94/33/EC on the protection of young people at work.
---------------------------	--

Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
---	---------------

Regulation (EC) No 850/2004 of the European Parliament and of the Council of 29 April 2004 on persistent organic pollutants and amending Directive 79/117/EEC	not regulated
---	---------------

Regulation (EC) No 689/2008 concerning the export and import of dangerous chemicals	not regulated
---	---------------

Substances of very high concern (SVHC)	This product does not contain substances of very high concern according to Regulation (EC) No 1907/2006 (REACH), Article 57 above the respective regulatory concentration limit of $\geq 0.1$ % (w/w).
--	--

*National legislation*

Storage class	10 - 13
---------------	---------

**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out.

---

**SECTION 16. Other information**

**Full text of H-Statements referred to under sections 2 and 3.**

H314	Causes severe skin burns and eye damage.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.
H400	Very toxic to aquatic life.

**Full text of R-phrases referred to under sections 2 and 3**

R34	Causes burns.
R37/38	Irritating to respiratory system and skin.
R41	Risk of serious damage to eyes.
R50	Very toxic to aquatic organisms.

**Training advice**

Provide adequate information, instruction and training for operators.

SAFETY DATA SHEET  
according to Regulation (EC) No. 1907/2006

Catalogue No. 822002  
Product name Crotonic anhydride (mixture of cis and trans isomers) for synthesis

**Labelling**

*Hazard pictograms*



*Signal word*

Danger

*Hazard statements*

H315 Causes skin irritation.  
H318 Causes serious eye damage.  
H335 May cause respiratory irritation.  
H400 Very toxic to aquatic life.

*Precautionary statements*

Prevention

P273 Avoid release to the environment.  
P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.  
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.  
P313 Get medical advice/ attention.

**Labelling (67/548/EEC or 1999/45/EC)**

<i>Symbol(s)</i>	Xi N	Irritant Dangerous for the environment
<i>R-phrases(s)</i>	37/38-41-50	Irritating to respiratory system and skin. Risk of serious damage to eyes. Very toxic to aquatic organisms.
<i>S-phrases(s)</i>	26-39-61	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear eye/face protection. Avoid release to the environment. Refer to special instructions/ Safety data sheets.

EC-No. 210-807-1

**Reduced labelling (≤125 ml)**

<i>Symbol(s)</i>	Xi N	Irritant Dangerous for the environment
<i>R-phrases(s)</i>	41	Risk of serious damage to eyes.
<i>S-phrases(s)</i>	26-39	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear eye/face protection.

**Key or legend to abbreviations and acronyms used in the safety data sheet**

Used abbreviations and acronyms can be looked up at [www.wikipedia.org](http://www.wikipedia.org).

**Regional representation**

This information is given on the authorised Safety Data Sheet for your country.

---

*The information contained herein is based on the present state of our knowledge. It characterises the product with regard to the appropriate safety precautions. It does not represent a guarantee of any properties of the product.*