

according to Regulation (EC) No. 1907/2006

Revision Date 26.06.2015

Version 5.5

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

#### 1.1 Product identifier

Catalogue No. 818256

Product name Cyclohexanecarboxylic acid chloride 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. 2719-27-9

# 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 (www.merckgroup.com).

# 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: prodsafe@merckgroup.com

1.4 Notrufnummer 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)

Acute toxicity, Category 4, Oral, H302 Skin corrosion, Category 1B, H314

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

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

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

Xn Harmful R22
C Corrosive R34
Xi Irritant R37

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





Signal word

according to Regulation (EC) No. 1907/2006

Catalogue No. 818256

Product name Cyclohexanecarboxylic acid chloride for synthesis

### Danger

### Hazard statements

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.

## Precautionary statements

Prevention

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

Response

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

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.

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

#### Reduced labelling (≤125 ml)

### Hazard pictograms





Signal word
Danger

### Hazard statements

H314 Causes severe skin burns and eye damage.

### Precautionary statements

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

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

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

CAS-No. 2719-27-9

#### 2.3 Other hazards

None known.

## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula C<sub>6</sub>H<sub>11</sub>COCl C<sub>7</sub>H<sub>11</sub>CIO (Hill)

EC-No. 220-322-7 Molar mass 146,62 g/mol

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

Chemical Name (Concentration)

CAS-No. Registration number Classification cyclohexanecarboxylic acid chloride (<= 100 %)

2719-27-9 \*)

Acute toxicity, Category 4, H302

according to Regulation (EC) No. 1907/2006

Catalogue No. 818256

Product name Cyclohexanecarboxylic acid chloride for synthesis

Skin corrosion, Category 1B, H314 Specific target organ toxicity - single exposure, Category 3, H335

\*) 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

cyclohexanecarboxylic acid chloride (<= 100 %)

2719-27-9 Xn, Harmful; R22

C, Corrosive; R34 Xi, Irritant; R37

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

General advice

First aider needs to protect himself.

After inhalation: fresh air. Call in physician.

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/shower. Call a physician immediately.

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

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

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

Irritation and corrosion, Cough, Shortness of breath Risk of blindness!

Nisk of billiariess:

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

No information available.

### **SECTION 5. Firefighting measures**

## 5.1 Extinguishing media

Suitable extinguishing media
Carbon dioxide (CO2), Dry powder

Unsuitable extinguishing media

Water, Foam

## 5.2 Special hazards arising from the substance or mixture

Combustible.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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Product name Cyclohexanecarboxylic acid chloride for synthesis

May not get in touch with:

Water

Caution! in contact with water product releases:

hydrochloric acid

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

Fire may cause evolution of:

Hydrogen chloride gas

## 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

Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. 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: Do not breathe vapours, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. 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 let product enter 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

Keep workplace dry. Do not allow product to come into contact with water.

Observe label precautions.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

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

according to Regulation (EC) No. 1907/2006

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Product name Cyclohexanecarboxylic acid chloride for synthesis

Dry. Tightly closed.

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: Viton (R)
Glove thickness: 0,70 mm
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber Glove thickness: 0,40 mm Break through time: > 120 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 890 Vitoject® (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).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Respirator.

The entrepeneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

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# Environmental exposure controls

Do not let product enter drains.

# SECTION 9. Physical and chemical properties

# 9.1 Information on basic physical and chemical properties

Form liquid

Colour colourless

Odour stinging

Odour Threshold No information available.

pH No information available.

Melting point No information available.

Boiling point/boiling range 180 - 181 °C

at 1.013 hPa

Flash point 66 °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 No information available.

Relative vapour density No information available.

Density 1,08 g/cm<sup>3</sup>

at 20 °C

Relative density No information available.

Water solubility at 20 °C

(decomposition)

Partition coefficient: n-

octanol/water

No information available.

Auto-ignition temperature No information available.

Decomposition temperature No information available.

Viscosity, dynamic No information available.

Explosive properties Not classified as explosive.

Oxidizing properties none

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### 9.2 Other data

none

## SECTION 10. Stability and reactivity

## 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

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

## 10.2 Chemical stability

sensitive to moisture

## 10.3 Possibility of hazardous reactions

Generates dangerous gases or fumes in contact with:

Water, Strong oxidizing agents

### 10.4 Conditions to avoid

Exposure to moisture Strong heating.

### 10.5 Incompatible materials

no information available

### 10.6 Hazardous decomposition products

in the event of fire: See section 5.

## **SECTION 11. Toxicological information**

### 11.1 Information on toxicological effects

Acute oral toxicity LD50 Rat: 965 mg/kg

(External MSDS)

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the oesophagus and the stomach.

absorption

Acute inhalation toxicity

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Acute dermal toxicity

This information is not available.

Skin irritation

Causes burns.

Eye irritation

Causes serious eye damage.

Risk of blindness!

Sensitisation

This information is not available.

Germ cell mutagenicity

according to Regulation (EC) No. 1907/2006

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Genotoxicity in vitro

Ames test

Result: negative

(calculated on the free acid)

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

**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.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

# **SECTION 12. Ecological information**

### 12.1 Toxicity

No information available.

### 12.2 Persistence and degradability

Biochemical Oxygen Demand (BOD)

1.600 mg/g (5 d)

(calculated on the free acid)

Chemical Oxygen Demand (COD)

2.750 mg/g

(calculated on the free acid)

## 12.3 Bioaccumulative potential

No information available.

## 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

Discharge into the environment must be avoided.

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Product name Cyclohexanecarboxylic acid chloride for synthesis

## **SECTION 13. Disposal considerations**

Waste treatment methods

See 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 3265

**14.2 Proper shipping name** CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.

(CYCLOHEXANE CARBOXYLIC ACID CHLORIDE)

**14.3 Class** 8

14.4 Packing group14.5 Environmentally hazardous

14.6 Special precautions for yes

user

Tunnel restriction code E

## Inland waterway transport (ADN)

Not relevant

Air transport (IATA)

**14.1 UN number** UN 3265

**14.2 Proper shipping name** CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.

(CYCLOHEXANE CARBOXYLIC ACID CHLORIDE)

**14.3 Class** 8

14.4 Packing group || 14.5 Environmentally becardage

14.5 Environmentally hazardous --14.6 Special precautions for no

user

Sea transport (IMDG)

**14.1 UN number** UN 3265

**14.2 Proper shipping name** CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.

(CYCLOHEXANE CARBOXYLIC ACID CHLORIDE)

**14.3 Class** 8

14.4 Packing group || 14.5 Environmentally hazardous --

14.6 Special precautions for

user

EmS F-A S-B

## 14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

yes

Not relevant

# **SECTION 15. Regulatory information**

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

EU regulations

according to Regulation (EC) No. 1907/2006

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Major Accident Hazard

Legislation

SEVESO III Not applicable

Occupational restrictions

Take note of Dir 94/33/EC on the protection of young people at work. Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where

applicable.

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 not regulated

and import of dangerous chemicals

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 8A

## 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.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.

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

R22 Harmful if swallowed.

R34 Causes burns.
R37 Irritating to respiratory system.

## Training advice

Provide adequate information, instruction and training for operators.

## Labelling

Hazard pictograms





according to Regulation (EC) No. 1907/2006

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Product name Cyclohexanecarboxylic acid chloride for synthesis

Signal word

Danger

Hazard statements

H227 Combustible liquid.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

H335 May cause respiratory irritation.

## Precautionary statements

Prevention

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

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

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

P308 + P310 IF exposed or concerned: immediately call a POISON CENTER or doctor/ physician.

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

Symbol(s)	C	Corrosive
R-phrase(s)	22-34-37	Harmful if swallowed. Causes burns. Irritating to respiratory system.
S-phrase(s)	26-36/37/39-45	In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek medical advice immediately (show

the label where possible).

EC-No. 220-322-7

Reduced labelling (≤125 ml)

Corrosive Symbol(s)

Harmful if swallowed. Causes burns. R-phrase(s) 22-34 26-36/37/39-45 S-phrase(s)

In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing, gloves and eye/face protection. In case of accident or if you feel unwell, seek

medical advice immediately (show the label where possible).

## 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.

# 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.