

according to Regulation (EC) No. 1907/2006

Revision Date 17.05.2018

Version 7.1

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

### 1.1 Product identifier

Catalogue No. 807059

Product name Diethyl oxalate 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. 95-92-1

#### 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 Emergency telephone Please contact the regional company representation in your country.

number

#### **SECTION 2. Hazards identification**

#### 2.1 Classification of the substance or mixture

# according to Regulation (EC) No. 1907/2006

Catalogue No. 807059

Product name Diethyl oxalate for synthesis

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

Acute toxicity, Category 4, Oral, H302

Skin corrosion, Category 1B, H314

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

#### 2.2 Label elements

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

## Hazard pictograms





Signal word

Danger

Hazard statements

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

### 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.

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





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Product name Diethyl oxalate for synthesis

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.

Contains: diethyl oxalate

*Index-No.* 607-147-00-5

#### 2.3 Other hazards

None known.

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

### 3.1 Substance

Formula  $C_2H_5OOCCOOC_2H_5$   $C_6H_{10}O_4$  (Hill)

Index-No. 607-147-00-5

EC-No. 202-464-1

Molar mass 146,14 g/mol

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

Chemical name (Concentration)

CAS-No. Registration number Classification

diethyl oxalate (<= 100 %)

95-92-1 \*)

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

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Product name Diethyl oxalate for synthesis

\*) 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.

#### 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. Remove contact lenses.

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

Risk of blindness!

Irritation and corrosion, Cough, Shortness of breath

Nausea, cardiovascular disorders, Headache

### 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

Water, Foam, Carbon dioxide (CO2), Dry powder

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Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Combustible.

Forms explosive mixtures with air on intense heating.

Vapours are heavier than air and may spread along floors.

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

#### 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. 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.

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# **SECTION 7. Handling and storage**

## 7.1 Precautions for safe handling

Advice on safe handling

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

Keep container tightly closed in a dry and well-ventilated place. Keep locked up or in an area accessible only to qualified or authorised persons.

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.

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#### 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: > 10 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).

Other protective equipment

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapours/aerosols are generated.

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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 oily

liquid

Colour colourless

Odour aromatic

Odour Threshold 0,1 ppm

pH No information available.

Melting point -41 °C

Boiling point/boiling range 185,7 °C

at 1.013 hPa

Flash point ca. 75 °C

at 1.013 hPa

Method: closed cup

Evaporation rate No information available.

Flammability (solid, gas) No information available.

Lower explosion limit 0,42 %(V)

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Product name Diethyl oxalate for synthesis

Upper explosion limit 2,67 %(V)

Vapour pressure 0,27 hPa

at 20 °C

Relative vapour density 5,04

(Air = 1.0)

Density 1,08 g/cm3

at 20 °C

Relative density No information available.

Water solubility at 20 °C

Method: OECD Test Guideline 105

(slow decomposition)

Partition coefficient: n- log Pow: 0,56

octanol/water (experimental)

(Lit.) Bioaccumulation is not expected.

Auto-ignition temperature No information available.

Decomposition temperature Distillable in an undecomposed state at normal pressure.

Viscosity, dynamic 2,17 mPa.s

at 20 °C

Explosive properties Not classified as explosive.

Oxidizing properties none

9.2 Other data

Ignition temperature 410 °C

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## **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

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

#### 10.3 Possibility of hazardous reactions

increased reactivity with:

strong oxidising agents, Strong bases, Strong acids, strong reducing agents, nitrates

#### 10.4 Conditions to avoid

Strong heating.

# 10.5 Incompatible materials

various plastics

## 10.6 Hazardous decomposition products

no information available

### **SECTION 11. Toxicological information**

# 11.1 Information on toxicological effects

Acute oral toxicity

LD50 Rat: 400 mg/kg

(calculated on the free acid) (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.

Acute inhalation toxicity

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

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Product name Diethyl oxalate for synthesis

Acute dermal toxicity

LD50 Rat: > 2.000 mg/kg OECD Test Guideline 402

Skin irritation

In vitro study

Result: Corrosive

**OECD Test Guideline 431** 

Causes burns.

Eye irritation

Causes serious eye damage.

Risk of blindness!

Sensitisation

Local lymph node assay (LLNA) Mouse

Result: negative

Method: OECD Test Guideline 429

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Escherichia coli/Salmonella typhimurium

Result: negative

Method: OECD Test Guideline 471

In vitro mammalian cell gene mutation test

Mouse lymphoma test

Result: negative

Method: OECD Test Guideline 476

Carcinogenicity

This information is not available.

Reproductive toxicity

This information is not available.

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Product name Diethyl oxalate for synthesis

Teratogenicity

This information is not available.

Specific target organ toxicity - single exposure

This information is not available.

Specific target organ toxicity - repeated exposure

This information is not available.

Aspiration hazard

This information is not available.

#### 11.2 Further information

After absorption:

Systemic effects:

cardiovascular disorders, Headache, Nausea, Reduction of the blood calcium concentration.

Toxic effect on:

Kidney

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 Poecilia reticulata (guppy): > 100 mg/l; 96 h

Analytical monitoring: yes OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates

semi-static test EC50 Daphnia magna (Water flea): > 100 mg/l; 48 h

Analytical monitoring: yes OECD Test Guideline 202

Toxicity to algae

static test ErC50 Desmodesmus subspicatus (green algae): 77,1 mg/l; 72 h

Analytical monitoring: yes OECD Test Guideline 201

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Catalogue No. 807059

Product name Diethyl oxalate for synthesis

Toxicity to bacteria

static test EC5 activated sludge: > 1.000 mg/l; 3 h

Analytical monitoring: yes OECD Test Guideline 209

#### 12.2 Persistence and degradability

Biodegradability

67,9 %; 28 d; aerobic

OECD Test Guideline 301D

The 10 day time window criterion is not fulfilled.

Readily biodegradable

### 12.3 Bioaccumulative potential

Partition coefficient: n-octanol/water

log Pow: 0,56 (experimental)

(Lit.) 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.

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Product name Diethyl oxalate 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 2525

14.2 Proper shipping name ETHYL OXALATE

**14.3 Class** 6.1

14.4 Packing group

14.5 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 2525

**14.2 Proper shipping name** ETHYL OXALATE

**14.3 Class** 6.1

14.4 Packing group

14.5 Environmentally hazardous --

**14.6 Special precautions for** no

user

Sea transport (IMDG)

# according to Regulation (EC) No. 1907/2006

Catalogue No. 807059

Product name Diethyl oxalate for synthesis

**14.1 UN number** UN 2525

**14.2 Proper shipping name** ETHYL OXALATE

**14.3 Class** 6.1

14.4 Packing group

14.5 Environmentally hazardous --

**14.6 Special precautions for** yes

user

EmS F-A S-A

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

Not relevant

#### **SECTION 15. Regulatory information**

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

EU regulations

Major Accident Hazard SEVESO III
Legislation 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 not regulated

deplete the ozone layer

Regulation (EC) No 850/2004 of the European not regulated

Parliament and of the Council of 29 April 2004 on

persistent organic pollutants and amending

Directive 79/117/EEC

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Product name Diethyl oxalate for synthesis

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 ≥ 0.1 % (w/w).

National legislation

Storage class 6.1C

### 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.

## Training advice

Provide adequate information, instruction and training for operators.

#### Labelling

Hazard pictograms





Signal word

Danger

Hazard statements

H227 Combustible liquid.

H302 Harmful if swallowed.

H314 Causes severe skin burns and eye damage.

# according to Regulation (EC) No. 1907/2006

Catalogue No. 807059

Product name Diethyl oxalate for synthesis

#### 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.

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.

Contains: diethyl oxalate

### 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.