

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Revision Date 17.05.2017

Version 10.0

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

### 1.1 Product identifier

Catalogue No. 800192

Product name Octanoic acid 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. 124-07-2

### 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](http://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](mailto:prodsafe@merckgroup.com)

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

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## SECTION 2. Hazards identification

### 2.1 Classification of the substance or mixture

Classification (REGULATION (EC) No 1272/2008)

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Skin corrosion, Category 1C, H314

Chronic aquatic toxicity, Category 3, H412

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*

H314 Causes severe skin burns and eye damage.

H412 Harmful to aquatic life with long lasting effects.

*Precautionary statements*

Prevention

P273 Avoid release to the environment.

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 ( $\leq 125$  ml)**

*Hazard pictograms*



*Signal word*

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Danger

## *Hazard statements*

H314 Causes severe skin burns and eye damage.  
H412 Harmful to aquatic life with long lasting effects.

## *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: Octanoic acid

*Index-No.* 607-708-00-4

## 2.3 Other hazards

None known.

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## SECTION 3. Composition/information on ingredients

### 3.1 Substance

Formula	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> COOH	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> (Hill)
Index-No.	607-708-00-4	
EC-No.	204-677-5	
Molar mass	144,21 g/mol	

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

#### *Chemical name (Concentration)*

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

124-07-2 \*)

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Chronic aquatic toxicity, Category 3, H412

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

## 3.2 Mixture

Not applicable

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## 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

Irritation and corrosion, Cough, Shortness of breath

Nausea, Vomiting, Headache, shock

Risk of blindness!

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

No information available.

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## SECTION 5. Firefighting measures

### 5.1 Extinguishing media

*Suitable extinguishing media*

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

## *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.

Vapours are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

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*

Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## 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. 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 and neutralising material (e.g. Chemisorb® H<sup>+</sup>, Merck Art. No. 101595). Dispose of properly. Clean up affected area.

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## 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.

#### *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.

Protective gas: nitrogen

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.

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## 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:	Nitrile rubber
Glove thickness:	0,40 mm
Break through time:	> 480 min

splash contact:

Glove material:	polychloroprene
Glove thickness:	0,65 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 730 Camatril® -Velours (full contact), KCL 720 Camapren® (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)).

### *Other protective equipment*

protective clothing

### *Respiratory protection*

required when vapours/aerosols are generated.

Recommended Filter type: Filter A-(P2)

The entrepreneur 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.

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## SECTION 9. Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

Form	liquid
Colour	light yellow
Odour	weak
Odour Threshold	No information available.
pH	3,5 at 0,5 g/l 20 °C
Melting point	16 °C
Boiling point/boiling range	237 °C at 1.013 hPa
Flash point	130 °C Method: open cup
Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	1 %(V)
Upper explosion limit	No information available.



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Vapour pressure	< 0,01 hPa at 20 °C
Relative vapour density	5,0
Density	0,908 - 0,912 g/cm <sup>3</sup> at 20,0 °C
Relative density	No information available.
Water solubility	0,68 g/l at 20 °C
Partition coefficient: n-octanol/water	log Pow: 3,05 (experimental) (Lit.) Bioaccumulation is not expected.
Auto-ignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	5,8 mPa.s at 20 °C
Explosive properties	Not classified as explosive.
Oxidizing properties	none

## 9.2 Other data

Ignition temperature	> 300 °C
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## SECTION 10. Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.

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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

Violent reactions possible with:

Strong oxidizing agents, bases, lithium aluminium hydride

## 10.4 Conditions to avoid

Strong heating.

## 10.5 Incompatible materials

no information available

## 10.6 Hazardous decomposition products

no information available

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## SECTION 11. Toxicological information

### 11.1 Information on toxicological effects

#### *Acute oral toxicity*

LD50 Rat: > 2.000 mg/kg

OECD Test Guideline 401

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*

LC50 Rat: > 0,162 mg/l; 4 h ; vapour

(ECHA)

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract, Inhalation may lead to the formation of oedemas in the respiratory tract., Symptoms may be delayed.

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## *Acute dermal toxicity*

This information is not available.

## *Skin irritation*

Rabbit

Result: Corrosive

OECD Test Guideline 404

Burns after prolonged exposure.

## *Eye irritation*

Causes serious eye damage.

Risk of blindness!

## *Sensitisation*

This information is not available.

## *Germ cell mutagenicity*

### *Genotoxicity in vitro*

Ames test

Salmonella typhimurium

Result: negative

(IUCLID)

## *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*

This information is not available.

## *Specific target organ toxicity - repeated exposure*

This information is not available.

## *Repeated dose toxicity*

Rat

male and female

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Oral

daily

NOAEL: 1.000 mg/kg

OECD Test Guideline 422

Subchronic toxicity

*Aspiration hazard*

This information is not available.

## 11.2 Further information

After uptake of large quantities:

Nausea, Vomiting, Headache, shock

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12. Ecological information

### 12.1 Toxicity

*Toxicity to fish*

semi-static test LC50 Danio rerio (zebra fish): 68 mg/l; 96 h

OECD Test Guideline 203

*Toxicity to daphnia and other aquatic invertebrates*

semi-static test EC50 Daphnia magna (Water flea): 13,4 mg/l; 48 h

OECD Test Guideline 202

The value is given in analogy to the following substances: Decanoic acid

*Toxicity to algae*

static test ErC50 Desmodesmus subspicatus (Scenedesmus subspicatus): 1,67 mg/l; 72 h

OECD Test Guideline 201

The value is given in analogy to the following substances: Decanoic acid

static test NOEC Desmodesmus subspicatus (Scenedesmus subspicatus): 0,47 mg/l; 72 h

OECD Test Guideline 201

The value is given in analogy to the following substances: Decanoic acid

*Toxicity to bacteria*

static test EC10 Pseudomonas putida: 912 mg/l; 18 h

ISO 10712

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## 12.2 Persistence and degradability

### *Biodegradability*

81 - 88 %; 28 d; aerobic

OECD Test Guideline 301F

Readily biodegradable

### *Theoretical oxygen demand (ThOD)*

2.440 mg/g

(Lit.)

## 12.3 Bioaccumulative potential

### *Partition coefficient: n-octanol/water*

log Pow: 3,05

(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

Discharge into the environment must be avoided.

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## 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.

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## 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. (OCTANOIC ACID)
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	yes
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. (OCTANOIC ACID)
14.3 Class	8
14.4 Packing group	III
14.5 Environmentally hazardous	--
14.6 Special precautions for user	no

### Sea transport (IMDG)

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<b>14.1 UN number</b>	UN 3265
<b>14.2 Proper shipping name</b>	CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (OCTANOIC ACID)
<b>14.3 Class</b>	8
<b>14.4 Packing group</b>	III
<b>14.5 Environmentally hazardous</b>	--
<b>14.6 Special precautions for user</b>	yes
<b>EmS</b>	F-A S-B
<b>14.7 Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code</b>	Not relevant

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## 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.
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Regulation (EC) No 1005/2009 on substances that deplete the ozone layer	not regulated
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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
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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).
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## *National legislation*

Storage class	8A
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## 15.2 Chemical safety assessment

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

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## SECTION 16. Other information

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

H314	Causes severe skin burns and eye damage.
H412	Harmful to aquatic life with long lasting effects.

### Training advice

Provide adequate information, instruction and training for operators.

### Labelling

#### *Hazard pictograms*



#### *Signal word*

Danger

#### *Hazard statements*

H314 Causes severe skin burns and eye damage.  
H412 Harmful to aquatic life with long lasting effects.

#### *Precautionary statements*

##### Prevention

P273 Avoid release to the environment.  
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

##### Response



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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: Octanoic acid

## 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.

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*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.*