

# SAFETY DATA SHEET

Version 6.8  
Revision Date 28.10.2024  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Octanoic acid

Product Number : C2875  
Brand : Sigma  
CAS-No. : 124-07-2

### 1.2 Other means of identification

Caprylic acid  
Acid C8

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other uses.

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

Company : Merck Life Science Ltd  
Level 26 PwC Tower, 15 Customs Street West  
1010 AUCKLAND  
NEW ZEALAND

Telephone : 0800 936 666  
E-mail address : customersupport.anz@merckgroup.com

### 1.5 Emergency telephone

Emergency Phone # : 0800 425 459 (CHEMTREC NZ)  
+64 9 801 0034 (Int'l CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 GHS Classification

Skin corrosion/irritation (Category 1C), H314  
Serious eye damage/eye irritation (Category 1), H318  
Hazardous to the aquatic environment - chronic hazard (Category 3), H412

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

### 2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word : Danger

Hazard Statements  
H314  
H412

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

## Precautionary Statements

### Prevention

P264	Wash skin thoroughly after handling.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.

### Response

P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.
P305 + P351 + P338 + P310	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

## 2.3 Other hazards - none

## SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

### 3.1 Substances

Synonyms : Caprylic acid  
Acid C8

Formula :  $C_8H_{16}O_2$   
Molecular weight : 144.21 g/mol  
CAS-No. : 124-07-2  
EC-No. : 204-677-5  
Index-No. : 607-708-00-4

### Hazardous ingredients

Component	Classification	Concentration
<b>Octanoic acid</b>		
	Skin Corr./Irrit. 1C; Eye Dam./Irrit. 1; Aquatic Chronic 3; H314, H318, H412	<= 100 %

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

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

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

**In case of eye contact**

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

**If swallowed**

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

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

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Carbon dioxide (CO<sub>2</sub>) Foam 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**

Carbon oxides

Combustible.

Vapors 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**

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

**5.4 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 vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection 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. Chemizorb® H<sup>+</sup>, Merck Art. No. 101595). Dispose of properly. Clean up affected area.

**6.4 Reference to other sections**

For disposal see section 13.

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## **SECTION 7: Handling and storage**

### **7.1 Precautions for safe handling**

For precautions see section 2.2.

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

#### **Storage conditions**

Tightly closed.

#### **Storage class**

Storage class (TRGS 510): 8A: Combustible, corrosive hazardous materials

### **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**

#### **Ingredients with workplace control parameters**

Contains no substances with occupational exposure limit values.

### **8.2 Exposure controls**

#### **Appropriate engineering controls**

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

#### **Personal protective equipment**

##### **Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

##### **Skin protection**

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 480 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0.65 mm

Break through time: 30 min

Material tested: KCL 720 Camapren®

##### **Body Protection**

protective clothing

**Respiratory protection**

required when vapours/aerosols are generated. Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

**Control of environmental exposure**

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**

a) Physical state	clear, viscous liquid
b) Color	light yellow
c) Odor	weak
d) Melting point/freezing point	Melting point/ range: 15 - 17 °C - lit.
e) Initial boiling point and boiling range	237 °C - lit.
f) Flammability (solid, gas)	No data available
g) Upper/lower flammability or explosive limits	Lower explosion limit: 1 %(V)
h) Flash point	> 110 °C - closed cup
i) Autoignition temperature	> 300 °C at 1,013 hPa
j) Decomposition temperature	No data available
k) pH	3.5 at 0.5 g/l
l) Viscosity	Viscosity, kinematic: 6.6 mm <sup>2</sup> /s at 20 °C - OECD Test Guideline 114 1144.08 mm <sup>2</sup> /s at 40 °C - OECD Test Guideline 114  Viscosity, dynamic: 6 mPa.s at 20 °C 5.8 mPa.s at 20 °C
m) Water solubility	0.68 g/l at 20 °C
n) Partition coefficient: n-octanol/water	log Pow: 3.05 - Bioaccumulation is not expected.
o) Vapor pressure	13 hPa at 124 °C
p) Density	0.91 g/cm <sup>3</sup> at 25 °C - lit.
Relative density	0.91 at 20 °C - OECD Test Guideline 109
q) Relative vapor density	4.98 - (Air = 1.0)
r) Particle characteristics	No data available
s) Explosive properties	Not classified as explosive.

t) Oxidizing properties none

## 9.2 Other safety information

Surface tension	33.7 mN/m at 0.6g/l at 23 °C - OECD Test Guideline 115
Dissociation constant	5.23 - 5.3 at 20 °C - OECD Test Guideline 112
Relative vapor density	4.98 - (Air = 1.0)

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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

Violent reactions possible with:  
Strong oxidizing agents  
bases  
lithium aluminium hydride

### 10.4 Conditions to avoid

Strong heating.

### 10.5 Incompatible materials

No data available

### 10.6 Hazardous decomposition products

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - > 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 esophagus and the stomach.

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.

LD50 Dermal - Rabbit - > 5,000 mg/kg

Remarks: (RTECS)

#### Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure - 4 h  
(OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

#### Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

**Respiratory or skin sensitization**

No data available

**Germ cell mutagenicity**

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster lung cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: negative

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 473

Result: Positive results were obtained in some in vitro tests.

**Carcinogenicity**

No data available

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**11.2 Additional Information**

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea, Vomiting, To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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	static test LC50 - <i>Lepomis macrochirus</i> (Bluegill sunfish) - 22 mg/l - 96 h (US-EPA)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - > 21 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - 43.73 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC10 - <i>Pseudomonas putida</i> - 912 mg/l - 18 h (ISO 10712)
Toxicity to fish(Chronic toxicity)	flow-through test LC50 - <i>Danio rerio</i> (zebra fish) - 9.8 mg/l - 28 d Remarks: (ECHA)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test LC50 - <i>Daphnia magna</i> (Water flea) - 20 mg/l - 21 d (OECD Test Guideline 211)

### 12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 30 d Result: > 72 % - Readily biodegradable. (OECD Test Guideline 301D)
Theoretical oxygen demand	2,440 mg/g Remarks: (Lit.)

### 12.3 Bioaccumulative potential

Bioaccumulation	<i>Danio rerio</i> (zebra fish) - 28 d at 21.5 °C - 3.6 mg/l(Octanoic acid)  Bioconcentration factor (BCF): 236 - 282 (OECD Test Guideline 305)
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### 12.4 Mobility in soil

No data available

### 12.5 Results of PBT and vPvB assessment

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

### 12.6 Endocrine disrupting properties

No data available

### 12.7 Other adverse effects

No data available



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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14: Transport information

### 14.1 UN number

ADR/RID: 3265

IMDG: 3265

IATA-DGR: 3265

### 14.2 UN proper shipping name

ADR/RID: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (Octanoic acid)  
(Octanoic acid)

IMDG: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (Octanoic acid)  
(Octanoic acid)

IATA-DGR: Corrosive liquid, acidic, organic, n.o.s. (Octanoic acid) (Octanoic acid)

### 14.3 Transport hazard class(es)

ADR/RID: 8

IMDG: 8

IATA-DGR: 8

### 14.4 Packaging group

ADR/RID: III

IMDG: III

IATA-DGR: III

### 14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA-DGR: no

### 14.6 Special precautions for user

None

### 14.7 Incompatible materials

#### Other regulations

Hazchem Code : 2X

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## SECTION 15: Regulatory information

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

#### National regulatory information

HSNO Approval Code:

HSNO Group Standard Approval: HSR002596 - Laboratory Chemicals and Reagent Kits  
Group Standard 2006

Tracking Required: not required

Approved Handler Cert.: not required

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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.

H318 Causes serious eye damage.

**Further information**

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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