SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name: Octanoic acid
Product Number: 153753
Brand: Aldrich
CAS-No.: 124-07-2

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

Identified uses: Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company: Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO  63103
UNITED STATES

Telephone: +1 314 771-5765
Fax: +1 800 325-5052

1.4 Emergency telephone

Emergency Phone #: 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Skin corrosion (Category 1C), H314
Serious eye damage (Category 1), H318
Short-term (acute) aquatic hazard (Category 3), H402
Long-term (chronic) aquatic 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 statement(s)
H314 Causes severe skin burns and eye damage.
H412 Harmful to aquatic life with long lasting effects.

Precautionary statement(s)
P264 Wash skin thoroughly after handling.
P273 Avoid release to the environment.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P330 + P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
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.
P363 Wash contaminated clothing before reuse.
P405 Store locked up.
P501 Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.1 Substances
Synonyms: Caprylic acid
          Acid C8

          Formula: C₈H₁₆O₂
          Molecular weight: 144.21 g/mol
          CAS-No.: 124-07-2
          EC-No.: 204-677-5

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Octanoic acid</td>
<td>Skin Corr. 1C; Eye Dam. 1; Aquatic Acute 3; Aquatic Chronic 3; H314, H318, H402, H412</td>
<td>&lt;= 100 %</td>
</tr>
</tbody>
</table>

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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media
Carbon dioxide (CO2) 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.

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⁺, Merck Art. No. 101595). Dispose of properly. Clean up affected area.

6.4 Reference to other sections
For disposal see section 13.

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

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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: 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.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

a) Appearance
   Form: clear, viscous liquid
   Color: light yellow

b) Odor
   weak

c) Odor Threshold
   No data available

d) pH
   3.5 at 0.5 g/l

e) Melting point/freezing point
   Melting point/range: 15 - 17 °C (59 - 63 °F) - lit.

f) Initial boiling point and boiling range
   237 °C 459 °F - lit.

g) Flash point
   > 110 °C (> 230 °F) - closed cup

h) Evaporation rate
   No data available

i) Flammability (solid, gas)
   No data available

j) Upper/lower flammability or explosive limits
   Lower explosion limit: 1 % (V)

k) Vapor pressure
   13 hPa at 124 °C (255 °F)

l) Vapor density
   4.98 - (Air = 1.0)

m) Density
   0.91 g/cm³ at 25 °C (77 °F) - lit.
   Relative density
   0.91 at 20 °C (68 °F) - OECD Test Guideline 109

n) Water solubility
   0.68 g/l at 20 °C (68 °F)

o) Partition coefficient:
   log Pow: 3.05 - Bioaccumulation is not expected.
n-octanol/water

p) Autoignition temperature > 300 °C (> 572 °F) at 1,013 hPa
q) Decomposition temperature No data available
r) Viscosity 6.6 mm²/s at 20 °C (68 °F) - OECD Test Guideline 114 - 4.08 mm²/s at 40 °C (104 °F) - OECD Test Guideline 114 - 
s) Explosive properties No data available
t) Oxidizing properties none

9.2 Other safety information

Surface tension 33.7 mN/m at 0.6g/l at 23 °C (73 °F) - OECD Test Guideline 115
Dissociation constant 5.23 - 5.3 at 20 °C (68 °F) - OECD Test Guideline 112
Relative vapor density 4.98 - (Air = 1.0)

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
Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5

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

**Serious eye damage/eye irritation**
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**
IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA’s list of regulated carcinogens.

**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. Cough, Shortness of breath, Headache, Nausea

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 - Lepomis macrochirus (Bluegill sunfish) - 22 mg/l - 96 h  
  (US-EPA)

- **Toxicity to daphnia and other aquatic invertebrates**  
  static test EC50 - Daphnia magna (Water flea) - > 21 mg/l - 48 h  
  (OECD Test Guideline 202)

- **Toxicity to algae**  
  static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 43.73 mg/l - 72 h  
  (OECD Test Guideline 201)

- **Toxicity to bacteria**  
  static test EC10 - Pseudomonas putida - 912 mg/l - 18 h  
  (ISO 10712)

#### 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**  
  Danio rerio (zebra fish) - 28 d  
  at 21.5 °C - 3.6 mg/l(Octanoic acid)

  Bioconcentration factor (BCF): 236 - 282  
  (OECD Test Guideline 305)
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

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 uncleansed containers like the product itself. 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
DOT (US)
UN number: 3265  Class: 8  Packing group: III
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (Octanoic acid)
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG
UN number: 3265  Class: 8  Packing group: III  EMS-No: F-A, S-B
Proper shipping name: CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S. (Octanoic acid)

IATA
UN number: 3265  Class: 8  Packing group: III
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (Octanoic acid)

SECTION 15: Regulatory information
SARA 302 Components
This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards
Acute Health Hazard

Massachusetts Right To Know Components
No components are subject to the Massachusetts Right to Know Act.
SECTION 16: Other information

Further information
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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