

SAFETY DATA SHEET

according to the OSHA
Hazard Communication Standard

Version 6.11
Revision Date 07/15/2026
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SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Octanoic acid-1-¹³C

Product Number : 296457
Brand : Aldrich
CAS-No. : 59669-16-8

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : Not Available

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 number

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

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Skin corrosion : Category 1C

Serious eye damage : Category 1

Short-term (acute) : Category 3

aquatic hazard

Long-term (chronic) aquatic hazard : Category 3

Other hazards

None known.

GHS label elements

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:**
P264 Wash skin thoroughly after handling.
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.
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.

Storage:
P405 Store locked up.

Disposal:
P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

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CAS-No. : 59669-16-8

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
Octanoic acid-1-13C	59669-16-8*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

- General advice : First aiders need to protect themselves.
Show this 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).
Call a physician immediately.
Do not attempt to neutralise.
- Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

SECTION 5. FIREFIGHTING MEASURES

- Suitable extinguishing media : Foam
Carbon dioxide (CO₂)
Dry powder
- Unsuitable extinguishing media : For this substance/mixture no limitations of extinguishing agents are given.

Specific hazards during fire fighting : 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.

Hazardous combustion products : Carbon oxides

Specific extinguishing methods : No data available

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

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

SECTION 6. ACCIDENTAL RELEASE MEASURES

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:
Wear appropriate personal protective equipment, as indicated in Section 8.

Environmental precautions : Do not let product enter drains.

Methods and materials : Cover drains. Collect, bind, and pump off spills.

for containment and cleaning up

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.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements

Further information on storage conditions : Tightly closed.

Storage class : 8A, Combustible, corrosive hazardous materials

Recommended storage temperature : Recommended storage temperature see product label.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type: : Filter type ABEK

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.

Hand protection

Remarks : required

Eye 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 and body protection	: protective clothing
Hygiene measures	: Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: liquid
Colour	: No data available
Odour	: No data available
Odour Threshold	: No data available
pH	: No data available
Melting point/ range	: 61 °F / 16 °C Method: lit.
Boiling point/boiling range	: 459 °F / 237 °C Method: lit.
Flash point	: 235 °F / 113 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapour pressure	: No data available
Relative vapour density	: No data available

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Relative density	: No data available
Density	: 0.91 g/mL (77 °F / 25 °C) 0.91 g/cm ³ (77 °F / 25 °C)
Water solubility	: No data available
Partition coefficient: n-octanol/water	: No data available
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available
Molecular weight	: 145.20 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

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.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Strong heating.
Incompatible materials	: No data available
Hazardous decomposition	: For Hazardous combustion products in the event of

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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)

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

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

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

Skin corrosion/irritation

Skin - Rabbit

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

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

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

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

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

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

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

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

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.

Remarks: The value is given in analogy to the following substances: Octanoic acid
Carcinogenicity

IARC: No component 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 component 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., 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.

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

Octanoic acid-1-13C:

Toxicity to fish : LC50 (Lepomis macrochirus (Bluegill sunfish)): 22

mg/l
 End point: mortality
 Exposure time: 96 h
 Test Type: static test
 Method: US-EPA
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: Octanoic acid

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): > 21 mg/l
 End point: Immobilization
 Exposure time: 48 h
 Test Type: static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 202
 GLP: yes
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: Octanoic acid

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata (green algae)): 43.73 mg/l
 Exposure time: 72 h
 Test Type: static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 201
 GLP: yes
 Remarks: The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: Octanoic acid

Toxicity to fish (Chronic toxicity) : LC50 (Danio rerio (zebra fish)): 9.8 mg/l
 End point: mortality
 Exposure time: 28 d
 Test Type: flow-through test
 Analytical monitoring: yes
 Remarks: (ECHA)
 The value is given in analogy to the following substances:
 The value is given in analogy to the following substances: Octanoic acid

Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity) : LC50 (Daphnia magna (Water flea)): 20 mg/l
 End point: mortality
 Exposure time: 21 d
 Test Type: semi-static test
 Analytical monitoring: yes
 Method: OECD Test Guideline 211
 GLP: yes

Remarks: The value is given in analogy to the following substances:

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

Toxicity to microorganisms

: EC10 (*Pseudomonas putida*): 912 mg/l

Exposure time: 18 h

Test Type: static test

Method: ISO 10712

GLP: yes

Remarks: The value is given in analogy to the following substances:

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

Ecotoxicology Assessment

Chronic aquatic toxicity : Harmful to aquatic life with long lasting effects.

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

Persistence and degradability

Components:

Octanoic acid-1-13C:

Biodegradability

: aerobic

Inoculum: Sewage sludge

Concentration: 5 mg/l

Result: Readily biodegradable.

Biodegradation: > 72 %

Exposure time: 30 d

Method: OECD Test Guideline 301D

Remarks: The value is given in analogy to the following substances:

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

Bioaccumulative potential

Components:

Octanoic acid-1-13C:

Bioaccumulation

: Species: *Danio rerio* (zebra fish)

Bioconcentration factor (BCF): 236 - 282

Exposure time: 28 d

Temperature: 70.7 °F / 21.5 °C

Concentration: 3.6 mg/l

Method: OECD Test Guideline 305

Remarks: The value is given in analogy to the following substances:

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

Mobility in soil

No data available

Other adverse effects

No data available

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS**Disposal methods**

Waste from residues : 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.

SECTION 14. TRANSPORT INFORMATION**International Regulations****IATA-DGR**

UN/ID No. : UN 3265
Proper shipping name : Corrosive liquid, acidic, organic, n.o.s.
(Octanoic acid-1-13C)
Class : 8
Packing group : III
Labels : Class 8 - Corrosive substances
Packing instruction (cargo : 856
aircraft)
Packing instruction : 852
(passenger aircraft)

IMDG-Code

UN number : UN 3265
Proper shipping name : CORROSIVE LIQUID, ACIDIC, ORGANIC, N.O.S.
(Octanoic acid-1-13C)
Class : 8
Packing group : III
Labels : 8
EmS Code : F-A, S-B
Marine pollutant : no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations**49 CFR**

UN/ID/NA number : UN 3265
Proper shipping name : Corrosive liquid, acidic, organic, n.o.s.

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(Octanoic acid-1-13C)
Class : 8
Packing group : III
Labels : Class 8 - Corrosive substances
ERG Code : 153
Marine pollutant : no
Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

SARA 311/312 Hazards : Acute Health Hazard

SARA 313 : 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.

US State Regulations

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Massachusetts Right To Know

No components are subject to the Massachusetts Right to Know Act.

Pennsylvania Right To Know

Octanoic acid-1-13C 59669-16-8

Maine Chemicals of High Concern

Product does not contain any listed chemicals

Vermont Chemicals of High Concern

Product does not contain any listed chemicals

Washington Chemicals of High Concern

Product does not contain any listed chemicals

The components of this product are reported in the following inventories:

US TSCA : Product contains substance(s) not listed on TSCA inventory.

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION**Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United

States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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