

SAFETY DATA SHEET

Version 6.3
Revision Date 04/11/2022
Print Date 06/01/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Octanoic acid-1-¹³C Extra

Product Number : 605832
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

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 : Octanoic acid-1-13C
Octanoic acid-1-13C
Caprylic acid-1-13C
Caprylic acid-1-13C

Formula : $^{13}\text{CC}_7\text{H}_{16}\text{O}_2$
Molecular weight : 145.20 g/mol
CAS-No. : 59669-16-8

Component	Classification	Concentration
Octanoic acid-1-13C Extra		
	Skin Corr. 1C; Eye Dam. 1; Aquatic Acute 3; Aquatic Chronic 3; H314, H318, H402, 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.

Aldrich - 605832

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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.

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**

Foam Carbon dioxide (CO₂) 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 material (e.g. Chemizorb®). 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

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: liquid
b) Odor	No data available
c) Odor Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: 16 °C (61 °F) - lit.
f) Initial boiling point and boiling range	237 °C 459 °F - lit.
g) Flash point	113 °C (235 °F) - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	No data available
k) Vapor pressure	No data available
l) Vapor density	No data available
m) Density	0.916 g/cm ³ at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	No data available
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

9.2 Other safety information

No data available

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) .
Stable

10.3 Possibility of hazardous reactions

No data available

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

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 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)

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
(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

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 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., 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:

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

Nausea

Vomiting

Headache

shock

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

Other dangerous properties can not be excluded.

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

Handle in accordance with good industrial hygiene and safety practice.

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

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) Remarks: The value is given in analogy to the following substances: Octanoic acid
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) Remarks: The value is given in analogy to the following substances: Octanoic acid
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - 43.73 mg/l - 72 h (OECD Test Guideline 201) Remarks: The value is given in analogy to the following substances: Octanoic acid
Toxicity to bacteria	static test EC10 - <i>Pseudomonas putida</i> - 912 mg/l - 18 h (ISO 10712) Remarks: The value is given in analogy to the following substances: Octanoic acid

12.2 Persistence and degradability

Biodegradability	aerobic - Exposure time 30 d Result: > 72 % - Readily biodegradable. (OECD Test Guideline 301D) Remarks: The value is given in analogy to the following substances: Octanoic acid
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12.3 Bioaccumulative potential

Bioaccumulation	<i>Danio rerio</i> (zebra fish) - 28 d at 21.5 °C - 3.6 mg/l (Octanoic acid-1-13C Extra) Bioconcentration factor (BCF): 236 - 282 (OECD Test Guideline 305) Remarks: The value is given in analogy to the following substances: Octanoic acid
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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

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. 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-1-13C Extra)
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-1-13C Extra)

IATA

UN number: 3265 Class: 8 Packing group: III
Proper shipping name: Corrosive liquid, acidic, organic, n.o.s. (Octanoic acid-1-13C Extra)
IATA Passenger: Not permitted for transport
IATA Cargo: Not permitted for transport

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.

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

Pennsylvania Right To Know Components

Octanoic acid-1-13C Extra

CAS-No.
59669-16-8

Revision Date

New Jersey Right To Know Components

Octanoic acid-1-13C Extra

CAS-No.
59669-16-8

Revision Date

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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