

Chemical Safety Data Sheet MSDS / SDS

OCTANOIC 1-13C ACID

Revision Date:2026-05-31 Revision Number:1

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

Product identifier

Product name : OCTANOIC 1-13C ACID
CBnumber : CB1472275
CAS : 59669-16-8
Synonyms : Caprylic Acid-1-13C,OCTANOIC ACID (1-13C)

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word Danger

Precautionary statements

P363 Wash contaminated clothing before reuse.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continuerinsing.
P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.
P280 Wear protective gloves/protective clothing/eye protection/face protection.
P273 Avoid release to the environment.

Hazard statements

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

SECTION 3: Composition/information on ingredients

Substance

Product name	: OCTANOIC 1-13C ACID
Synonyms	: Caprylic Acid-1-13C,OCTANOIC ACID (1-13C)
CAS	: 59669-16-8
MF	: C ₈ H ₁₆ O ₂
MW	: 145.22

SECTION 4: 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). 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) 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. 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.

Hazardous combustion products

Carbon oxides

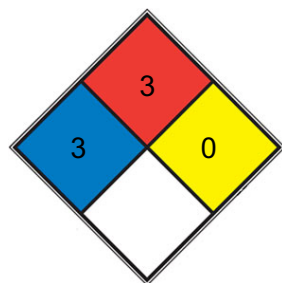
Specific extinguishing methods

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.

NFPA 704



HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

FIRE 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N₂](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

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. Advice for emergency responders: For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

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.

SECTION 7: Handling and storage

Handling

For precautions see section 2.2.

Storage

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.

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 and body protection

protective clothing

Hand protection

Remarks

required

Hygiene measures

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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

liquid

Color

No data available

Odor

No data available

Odor Threshold

No data available

pH

No data available

Melting point/ range

16 °C

Method: lit.

Boiling point/boiling range

237 °C

Method: lit.

Flash point

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

Vapor pressure

No data available

Relative vapor density

No data available

Relative density

0.910 g/mL at 25 °C

Density

0.91 g/mL (25 °C) 0.91 g/cm³ (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

Solubility

DMF: 30 mg/ml; DMSO: 30 mg/ml; Ethanol: 30 mg/ml

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 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

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

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

Classified based on available data. For more details, see section 2

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 ac- idTest 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 ac- idTest 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 ac- idTest 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 ac- idCarcinogenicity

No data available

Reproductive toxicity

Classified based on available data. For more details, see section 2

Specific target organ toxicity - single exposure

Classified based on available data. For more details, see section 2

Specific target organ toxicity - repeated exposure

Classified based on available data. For more details, see section 2

Aspiration hazard

Classified based on available data. For more details, see section 2

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.

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: 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

SECTION 13: Disposal considerations

Disposal methods

Waste from residues

Offer surplus and non-recyclable solutions to a licensed disposal company.

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 aircraft) : 856

Packing instruction (passenger aircraft) : 852

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 Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.
National regulation

JT/T 617

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
Environmentally hazardous : 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

National regulatory information

Regulations on Safety Management of Hazardous Chemicals

Catalogue of Hazardous Chemicals

Hazardous Chemicals for Priority Management

under SAWS

China. List of Explosive Precursors

Not applicable

Regulation of Environmental Management on the First Import of Chemicals and the Import and Export of Toxic Chemicals

China Severely Restricted Toxic Chemicals for Import and Export

SECTION 16: Other information

Full text of other abbreviations

AIRC - Australian Inventory of Industrial Chemicals

ANTT - National Agency for Transport by Land of Brazil

ASTM - American Society for the Testing of Materials

bw - Body weight

CMR - Carcinogen, Mutagen or Reproductive Toxicant

DIN - Standard of the German Institute for Standardisation

DSL - Domestic Substances List (Canada)

EC_x - Concentration associated with x% response

EL_x - Loading rate associated with x% response

EmS - Emergency Schedule

ENCs - Existing and New Chemical Substances (Japan)

ErC_x - Concentration associated with x% growth rate response

ERG - Emergency Response Guide

GHS - Globally Harmonized System

GLP - Good Laboratory Practice

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 Organization

ISHL - Industrial Safety and Health Law (Japan)

ISO - International Organisation for Standardization

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

n.o.s. - Not Otherwise Specified

NCh - Chilean Norm

NO(A)EC - No Observed (Adverse) Effect Concentration

NO(A)EL - No Observed (Adverse) Effect Level

NOELR - No Observable Effect Loading Rate

NOM - Official Mexican Norm

NTP - National Toxicology Program

NZIoC - New Zealand Inventory of Chemicals

OECD - Organization 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

REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals

SADT - Self-Accelerating Decomposition Temperature

SDS - Safety Data Sheet

TCSI - Taiwan Chemical Substance Inventory

TDG - Transportation of Dangerous Goods

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

WHMIS - Workplace Hazardous Materials Information System

Disclaimer:

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.