

Safety Data Sheet acc. to OSHA HCS

Date of issue: 01/30/2025

Revision date 01/30/2025

1 Identification

- **Product identifier**
- **Trade name: Octanoic Acid-13C**
- **Synonym** octanoic-1-13C acid; Caprylic Acid-13C; FA 8:0-13C
- **Other means of identification**
- **Article number:** 29461
- **Application of the substance / the mixture**
This product is for research use - Not for human or veterinary diagnostic or therapeutic use.
- **Details of the supplier of the safety data sheet**
- **Manufacturer/Supplier:**
Cayman Chemical Co.
1180 E. Ellsworth Rd.
Ann Arbor, MI 48108
USA
- **Information department:** Product safety department
- **Emergency telephone number:**
During normal opening times: +1 (734) 971-3335
US/CANADA: 800-424-9300
Outside US/CANADA: 703-741-5970

2 Hazard(s) identification

- **Classification of the substance or mixture**



GHS02 Flame

Flammable liquids 2 H225 Highly flammable liquid and vapor.



GHS05 Corrosion

Skin corrosion 1B H314 Causes severe skin burns and eye damage.
Eye damage 1 H318 Causes serious eye damage.

- **Label elements**
- **GHS label elements**

The product is classified and labeled according to the Globally Harmonized System (GHS).

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- **Hazard pictograms**



GHS02 GHS05

- **Signal word** Danger

- **Hazard-determining components of labeling:**

Octanoic Acid-13C

- **Hazard statements**

H225 Highly flammable liquid and vapor.

H314 Causes severe skin burns and eye damage.

- **Precautionary statements**

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources.
No smoking.

P233 Keep container tightly closed.

P240 Ground / bond container and receiving equipment.

P241 Use explosion-proof [electrical/ventilating/lighting] equipment.

P242 Use non-sparking tools.

P243 Take action to prevent static discharge.

P260 Do not breathe dusts or mists.

P264 Wash thoroughly after handling.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing 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 [or shower].

P304+P340 If inhaled: Remove person to fresh air and keep comfortable for breathing.

P305+P351+P338 If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P310 Immediately call a poison center/doctor.

P321 Specific treatment (see on this label).

P363 Wash contaminated clothing before reuse.

P370+P378 In case of fire: Use CO₂, powder or water spray to extinguish.

P403+P235 Store in a well-ventilated place. Keep cool.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

- **Information pertaining to particular dangers for man and environment:**

- **Classification system:**

- **NFPA ratings (scale 0 - 4)**



Health = 3

Fire = 3

Reactivity = 0

- **HMIS-ratings (scale 0 - 4)**



HEALTH 3 Health = 3

FIRE 3 Fire = 3

REACTIVITY 0 Reactivity = 0

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- **Other hazards**
- **Results of PBT and vPvB assessment**
- **PBT:** Not applicable.
- **vPvB:** Not applicable.
- **Classification according to (d)(1)(ii) of § 1910.1200**
The SDS issuer does not object to the classifications provided by importers or manufacturers of precursor products.
- **Hazards not otherwise classified**
There are no adverse physical or health effects known that are not covered by the hazard classes of the Hazard Communications Standard.

3 Composition/information on ingredients

- **Chemical characterization: Mixtures**
- **Description:** Mixture of the substances listed below with nonhazardous additions.

- **Dangerous components:**

CAS: 64-17-5 RTECS: KQ6300000	ethanol	75.0%
CAS: 59669-16-8	Octanoic Acid-13C	25.0%

4 First-aid measures

- **Description of first aid measures**
- **General information:** Immediately remove any clothing soiled by the product.
- **After inhalation:** In case of unconsciousness place patient stably in side position for transportation.
- **After skin contact:** Immediately wash with water and soap and rinse thoroughly.
- **After eye contact:** Rinse opened eye for several minutes under running water. Then consult a doctor.
- **After swallowing:** Drink copious amounts of water and provide fresh air. Immediately call a doctor.
- **Most important symptoms and effects, both acute and delayed**
No further relevant information available.
- **Indication of any immediate medical attention and special treatment needed**
No further relevant information available.

5 Fire-fighting measures

- **Extinguishing media**
- **Suitable extinguishing agents:**
CO₂, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
- **Special hazards arising from the substance or mixture**
67-56-1 During heating or in case of fire poisonous gases are produced.
- **Advice for firefighters**
- **Protective equipment:** Mouth respiratory protective device.

6 Accidental release measures

- **Personal precautions, protective equipment and emergency procedures**
Mount respiratory protective device.
Wear protective equipment. Keep unprotected persons away.

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- **Environmental precautions:**
Dilute with plenty of water.
Do not allow to enter sewers/ surface or ground water.
- **Methods and material for containment and cleaning up:**
Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).
Use neutralizing agent.
Dispose contaminated material as waste according to section 13.
Ensure adequate ventilation.
- **Protective Action Criteria for Chemicals**

· **PAC-1:**

64-17-5	ethanol	1,800 ppm
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· **PAC-2:**

64-17-5	ethanol	3300* ppm
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· **PAC-3:**

64-17-5	ethanol	15000* ppm
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· **Reference to other sections**

- See Section 7 for information on safe handling.
- See Section 8 for information on personal protection equipment.
- See Section 13 for disposal information.

7 Handling and storage

- **Precautions for safe handling**
Ensure good ventilation/exhaustion at the workplace.
Prevent formation of aerosols.
- **Information about protection against explosions and fires:**
Keep ignition sources away - Do not smoke.
Protect against electrostatic charges.
Keep respiratory protective device available.
- **Conditions for safe storage, including any incompatibilities**
- **Storage:** Store in accordance with information listed on the product insert.
- **Requirements to be met by storerooms and receptacles:** Store in a cool location.
- **Information about storage in one common storage facility:** Not required.
- **Further information about storage conditions:**
Keep receptacle tightly sealed.
Store in cool, dry conditions in well sealed receptacles.
- **Specific end use(s)** No further relevant information available.

8 Exposure controls/personal protection

- **Control parameters**
- **Components with limit values that require monitoring at the workplace:**
The following constituent is the only constituent of the product which has a PEL, TLV or other recommended exposure limit.
At this time, the remaining constituent has no known exposure limits.

64-17-5 ethanol

PEL	Long-term value: 1900 mg/m ³ , 1000 ppm
REL	Long-term value: 1900 mg/m ³ , 1000 ppm

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TLV	Short-term value: 1000 ppm A3
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- **Additional information:** The lists that were valid during the creation were used as basis.
- **Exposure controls**
- **Appropriate engineering controls** No further data; see section 7.
- **Personal protective equipment:**
- **General protective and hygienic measures:**
Keep away from foodstuffs, beverages and feed.
Immediately remove all soiled and contaminated clothing.
Wash hands before breaks and at the end of work.
Avoid contact with the eyes.
Avoid contact with the eyes and skin.
- **Breathing equipment:**
In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.
- **Protection of hands:**



Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation. Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

- **Material of gloves**
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.
- **Penetration time of glove material**
The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.
- **Eye protection:**



Tightly sealed goggles

9 Physical and chemical properties

Information on basic physical and chemical properties

- **General Information**
- **Physical state** Liquid
- **Color:** According to product specification
- **Odor:** Characteristic
- **Structural Formula** C7[13C]H16O2
- **Molecular Weight** 145.2 g/mol
- **Storage Buffer**
- **Odor threshold:** Not determined.

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· Formulation	A solution in ethanol
· Melting point/Melting range:	Undetermined.
· Boiling point/Boiling range:	78 °C (172.4 °F)
· Flammability:	Highly flammable.
· Explosion limits:	
· Lower:	3.3 Vol %
· Upper:	19 Vol %
· Flash point:	13 °C (55.4 °F)
· Auto igniting:	425 °C (797 °F)
· Decomposition temperature:	Not determined.
· pH-value:	Not determined.
· Viscosity:	
· Kinematic:	Not determined.
· SOLUBILITY	DMF: 30 mg/ml; DMSO: 30 mg/ml; Ethanol: 30 mg/ml
· Dynamic:	Not determined.
· Solubility in / Miscibility with	
· Water:	Fully miscible.
· Partition coefficient (n-octanol/water):	Not determined.
· Vapor pressure at 20 °C (68 °F):	59 hPa (44.3 mm Hg)
· Vapor pressure at 50 °C (122 °F):	280 hPa (210 mm Hg)
· Density:	Not determined.
· Relative density	Not determined.
· Vapor density	Not determined.
· Particle characteristics	Not applicable.
· Other information	
· Appearance:	
· Form:	Liquid
· Important information on protection of health and environment, and on safety.	
· Ignition temperature:	Product is not selfigniting.
· Danger of explosion:	Product is not explosive. However, formation of explosive air/vapor mixtures are possible.
· Solvent content:	
· Organic solvents:	75.0 %
· VOC content:	75.00 %
	750.0 g/l / 6.26 lb/gal
· Solids content:	0.0 %
· Change in condition	
· Evaporation rate	Not determined.

10 Stability and reactivity

- **Reactivity** No further relevant information available.
- **Chemical stability**
- **Thermal decomposition / conditions to be avoided:**
No decomposition if used according to specifications.
- **Possibility of hazardous reactions** No dangerous reactions known.
- **Conditions to avoid** No further relevant information available.
- **Incompatible materials:** strong acids, strong bases, oxidizing agents

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· **Hazardous decomposition products:** carbon oxides

11 Toxicological information

· **Information on toxicological effects**· **Acute toxicity:**· **LD/LC50 values that are relevant for classification:**

64-17-5 ethanol

Oral	LD50	10,470 mg/kg (rat) OECD Test Guideline 401
Inhalative	LC50/4 h	117–125 mg/l (rat) OECD 403 (rat)

· **Primary irritant effect:**· **on the skin:** Caustic effect on skin and mucous membranes.· **on the eye:**

Strong caustic effect.

Strong irritant with the danger of severe eye injury.

· **Sensitization:** No sensitizing effects known.· **Additional toxicological information:**

The product shows the following dangers according to internally approved calculation methods for preparations:

Corrosive

Irritant

Swallowing will lead to a strong caustic effect on mouth and throat and to the danger of perforation of esophagus and stomach.

· **Interactive effects** No interactive effects between components are known.· **Carcinogenic categories**· **IARC (International Agency for Research on Cancer)**

64-17-5	ethanol	1
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· **NTP (National Toxicology Program)**

None of the ingredients is listed.

· **OSHA-Ca (Occupational Safety & Health Administration)**

None of the ingredients is listed.

· **Alternative sources for toxicological information**

No non-standard sources for toxicological information where used.

12 Ecological information

· **Toxicity**· **Aquatic toxicity:** No further relevant information available.· **Persistence and degradability** No further relevant information available.· **Bioaccumulative potential** No further relevant information available.· **Mobility in soil** No further relevant information available.· **Results of PBT and vPvB assessment**· **PBT:** Not applicable.· **vPvB:** Not applicable.

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- **Other adverse effects**
- **Additional ecological information:**
- **General notes:**
 Water hazard class 1 (Self-assessment): slightly hazardous for water
 Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
 Must not reach bodies of water or drainage ditch undiluted or unneutralized.

13 Disposal considerations

- **Waste treatment methods**
- **Recommendation:**
 Must not be disposed of together with household garbage. Do not allow product to reach sewage system.
- **Uncleaned packagings:**
- **Recommendation:** Disposal must be made according to official regulations.
- **Recommended cleansing agent:** Water, if necessary with cleansing agents.

14 Transport information

- **UN-Number**
- **DOT, IMDG, IATA** UN2924
- **UN proper shipping name**
- **DOT** Flammable liquids, corrosive, n.o.s. (Ethanol, Octanoic Acid-13C)
- **IMDG** FLAMMABLE LIQUID, CORROSIVE, N.O.S. (ETHANOL (ETHYL ALCOHOL), Octanoic Acid-13C)
- **IATA** Flammable liquid, corrosive, n.o.s. (ETHANOL, Octanoic Acid-13C)
- **Transport hazard class(es)**
- **DOT**
- 
- **Class** 3 Flammable liquids
- **Label** 3, 8
- **IMDG**
- 
- **Class** 3 Flammable liquids

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· Label	3/8
· IATA	
	
· Class	3 Flammable liquids
· Label	3 (8)
· Packing group	
· DOT, IMDG, IATA	II
· Environmental hazards:	Not applicable.
· Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
· Transport/Additional information:	
· DOT	
· Quantity limitations	On passenger aircraft/rail: 1 L On cargo aircraft only: 5 L
· IMDG	
· Limited quantities (LQ)	1L
· Excepted quantities (EQ)	Code: E2 Maximum net quantity per inner packaging: 30 ml Maximum net quantity per outer packaging: 500 ml
· IATA	
· Remarks:	When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of E1, E2, E4, or E5, this item meets the De Minimis Quantities exemption, per IATA 2.6.10. Therefore packaging does not have to be labeled as Dangerous Goods/Excepted Quantity.
· Special precautions for user	Warning: Flammable liquids
· Hazard identification number (Kemler code):	338
· EMS Number:	F-E,S-C
· Segregation groups	(SGG1) Acids
· Stowage Category	B
· Stowage Code	SW2 Clear of living quarters.
· UN "Model Regulation":	UN 2924 FLAMMABLE LIQUID, CORROSIVE, N.O.S. (ETHANOL (ETHYL ALCOHOL), OCTANOIC ACID-13C), 3 (8), II

15 Regulatory information

- Safety, health and environmental regulations/legislation specific for the substance or mixture
No further relevant information available.

- Sara

- Section 355 (extremely hazardous substances):

None of the ingredients is listed.

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· Section 313 (Specific toxic chemical listings):
None of the ingredients is listed.

· TSCA (Toxic Substances Control Act):
64-17-5 ethanol
ACTIVE

· Hazardous Air Pollutants
None of the ingredients is listed.

· Chemicals known to cause cancer:
None of the ingredients is listed.

· Chemicals known to cause reproductive toxicity for females:
None of the ingredients is listed.

· Chemicals known to cause reproductive toxicity for males:
None of the ingredients is listed.

· Chemicals known to cause developmental toxicity:
64-17-5 ethanol

· Carcinogenic categories
· EPA (Environmental Protection Agency)
None of the ingredients is listed.

· TLV (Threshold Limit Value)
64-17-5 ethanol
A3

· NIOSH-Ca (National Institute for Occupational Safety and Health)
None of the ingredients is listed.

· Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

16 Other information

All chemicals may pose unknown hazards and should be used with caution. This SDS applies only to the material as packaged. If this product is combined with other materials, deteriorates, or becomes contaminated, it may pose hazards not mentioned in this SDS. Cayman Chemical Company assumes no responsibility for incidental or consequential damages, including lost profits, arising from the use of these data. It shall be the user's responsibility to develop proper methods of handling and personal protection based on the actual conditions of use. While this SDS is based on technical data judged to be reliable, Cayman Chemical Company assumes no responsibility for the completeness or accuracy of the information contained herein.

- **Department issuing SDS:** Environment protection department.

- **Contact:** -

- **Date of previous version** 04/20/2022

- **Date of preparation** 01/30/2025

- **Abbreviations and acronyms:**

- IMDG: International Maritime Code for Dangerous Goods

- DOT: US Department of Transportation

- IATA: International Air Transport Association

- EINECS: European Inventory of Existing Commercial Chemical Substances

- ELINCS: European List of Notified Chemical Substances

- CAS: Chemical Abstracts Service (division of the American Chemical Society)

- NFPA: National Fire Protection Association (USA)

- HMIS: Hazardous Materials Identification System (USA)

- VOC: Volatile Organic Compounds (USA, EU)

- LC50: Lethal concentration, 50 percent

- LD50: Lethal dose, 50 percent

- PBT: Persistent, Bioaccumulative and Toxic

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vPvB: very Persistent and very Bioaccumulative
NIOSH: National Institute for Occupational Safety
OSHA: Occupational Safety & Health
TLV: Threshold Limit Value
PEL: Permissible Exposure Limit
REL: Recommended Exposure Limit
Flammable liquids 2: Flammable liquids – Category 2
Skin corrosion 1B: Skin corrosion/irritation – Category 1B
Eye damage 1: Serious eye damage/eye irritation – Category 1
· *** Data compared to the previous version altered.**

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