

SAFETY DATA SHEET

Version 6.4
Revision Date 08/30/2023
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SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Acetic acid-1-¹³C

Product Number : 279285
Brand : Aldrich
CAS-No. : 1563-79-7

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)**

Flammable liquids (Category 3), H226
Skin corrosion (Category 1A), H314
Serious eye damage (Category 1), H318

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)	
H226	Flammable liquid and vapor.
H314	Causes severe skin burns and eye damage.
Precautionary statement(s)	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242	Use only non-sparking tools.
P243	Take precautionary measures against static discharge.
P264	Wash skin thoroughly after handling.
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.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.
P403 + P235	Store in a well-ventilated place. Keep cool.
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

Formula	: $^{13}\text{CCH}_4\text{O}_2$
Molecular weight	: 61.04 g/mol
CAS-No.	: 1563-79-7
EC-No.	: 625-762-7

Component	Classification	Concentration
Acetic acid-1-13C		
	Flam. Liq. 3; Skin Corr. 1A; Eye Dam. 1; H226, H314, H318	<= 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.

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

Water 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 at elevated temperatures.

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

Remove container from danger zone and cool with water. 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. Keep away from heat and sources of ignition. 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. Risk of explosion.

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

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Store under inert gas. hygroscopic

Storage class

Storage class (TRGS 510): 3: Flammable liquids

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

Component	CAS-No.	Value	Control parameters	Basis
Acetic acid-1-13C	1563-79-7	TWA	10 ppm	USA. ACGIH Threshold Limit Values (TLV)
		STEL	15 ppm	USA. ACGIH Threshold Limit Values (TLV)
		TWA	10 ppm 25 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	15 ppm 37 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	10 ppm 25 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	10 ppm 25 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		C	40 ppm	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	15 ppm 37 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		TWA	10 ppm 25 mg/m3	USA. Table Z-1-A Limits for Air Contaminants (1989 vacated 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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Latex gloves

Minimum layer thickness: 0.6 mm

Break through time: 30 min

Material tested: Lapren® (KCL 706 / Aldrich Z677558, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: filter E-(P2)

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.

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. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: clear, liquid
Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: 16.2 °C (61.2 °F) |
| f) Initial boiling point and boiling range | 117 - 118 °C 243 - 244 °F at 1,013 hPa |
| g) Flash point | 40 °C (104 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 19.9 %(V)
Lower explosion limit: 4 %(V) |
| k) Vapor pressure | 15.2 hPa at 20 °C (68 °F) |

l) Vapor density	2.11 - (Air = 1.0)
m) Density	1.060 g/cm ³
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	none

9.2 Other safety information

Relative vapor density	2.11 - (Air = 1.0)
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SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Risk of explosion with:

Strong oxidizing agents

peroxi compounds

perchloric acid

chromosulfuric acid

nitrates

fuming sulfuric acid

phosphorus halides

hydrogen peroxide

chromium(VI) oxide

potassium permanganate

Violent reactions possible with:

Metals

Iron

Zinc

magnesium

alkali hydroxides

nonmetallic halides

ethanolamine

Aldehydes

Alcohols
halogen-halogen compounds
chlorosulfonic acid
strong alkalis
Nitric acid
chromosulfuric acid
Potassium hydroxide
Risk of ignition or formation of inflammable gases or vapours with:
Metals
Iron
Zinc
magnesium
Mild steel
Possible formation of:
Hydrogen

10.4 Conditions to avoid

Exposure to moisture.
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 - 3,310 mg/kg

Remarks: (RTECS)

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

LC50 Inhalation - Mouse - 4 h - 2,819 mg/l - vapor

Remarks: (RTECS)

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

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Causes burns. - 4 h

(OECD Test Guideline 404)

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes burns. - 4 h

(OECD Test Guideline 405)

Remarks: (IUCLID)

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

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: 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: acetic acid
Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary 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: acetic acid

Test Type: Micronucleus test

Species: Rat

Cell type: Bone marrow

Application Route: inhalation (vapor)

Method: Mutagenicity (micronucleus test)

Result: negative

Remarks: The value is given in analogy to the following substances: acetic 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, Ingestion or inhalation of concentrated acetic acid causes damage to tissues of the respiratory and digestive tracts. Symptoms include: hematemesis, bloody diarrhea, edema and/or perforation of the esophagus and pylorus, pancreatitis, hematuria, anuria, uremia, albuminuria, hemolysis, convulsions, bronchitis, pulmonary edema, pneumonia,

cardiovascular collapse, shock, and death. Direct contact or exposure to high concentrations of vapor with skin or eyes can cause: erythema, blisters, tissue destruction with slow healing, skin blackening, hyperkeratosis, fissures, corneal erosion, opacification, iritis, conjunctivitis, and possible blindness.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Kidney - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish	semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - > 1,000 mg/l - 96 h (OECD Test Guideline 203) Remarks: The value is given in analogy to the following substances: acetic acid
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - > 1,000 mg/l - 48 h (OECD Test Guideline 202) Remarks: The value is given in analogy to the following substances: acetic acid
Toxicity to algae	static test EC50 - Skeletonema costatum - > 1,000 mg/l - 72 h (ISO 10253) Remarks: The value is given in analogy to the following substances: acetic acid
Toxicity to bacteria	EC5 - Pseudomonas putida - 2,850 mg/l - 16 h Remarks: neutral (maximum permissible toxic concentration) (Lit.) The value is given in analogy to the following substances: acetic acid
	microtox test EC50 - Photobacterium phosphoreum - 11 mg/l - 15 min Remarks: (IUCLID) The value is given in analogy to the following substances: acetic acid

12.2 Persistence and degradability

Biodegradability	Result: 99 % - Readily biodegradable. (OECD Test Guideline 301D) Remarks: (HSDB) The value is given in analogy to the following substances: acetic acid
	Result: 95 % - Readily eliminated from water

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(OECD Test Guideline 302B)
Remarks: The value is given in analogy to the following substances:
acetic acid

12.3 Bioaccumulative potential

No data available

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.

SECTION 14: Transport information

DOT (US)

UN number: 2789 Class: 8 (3) Packing group: II
Proper shipping name: Acetic acid, glacial
Reportable Quantity (RQ): 5000 lbs
Poison Inhalation Hazard: No

IMDG

UN number: 2789 Class: 8 (3) Packing group: II EMS-No: F-E, S-C
Proper shipping name: ACETIC ACID, GLACIAL

IATA

UN number: 2789 Class: 8 (3) Packing group: II
Proper shipping name: Acetic acid, glacial

SECTION 15: Regulatory information

SARA 302 Components

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

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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

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components

Acetic acid-1-13C	CAS-No. 1563-79-7	Revision Date 1993-04-24
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Pennsylvania Right To Know Components

Acetic acid-1-13C	CAS-No. 1563-79-7	Revision Date 1993-04-24
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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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