

## SAFETY DATA SHEET

Version 6.4  
Revision Date 09/17/2021  
Print Date 06/01/2022

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

Product name : Acetonitrile- $^{13}\text{C}_2$

Product Number : 485217  
Brand : Aldrich  
CAS-No. : 1722-25-4

**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 2), H225  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 4), H332  
Acute toxicity, Dermal (Category 4), H312  
Eye irritation (Category 2A), H319

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

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Hazard statement(s)	
H225	Highly flammable liquid and vapor.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H319	Causes serious eye irritation.
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.
P261	Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P280	Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
P305 + P351 + P338	IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P337 + P313	If eye irritation persists: Get medical advice/ attention.
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.
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	: Methyl cyanide-13C2
Formula	: $^{13}\text{C}_2\text{H}_3\text{N}$
Molecular weight	: 43.02 g/mol
CAS-No.	: 1722-25-4

Component	Classification	Concentration
<b>Acetonitrile-13C2</b>		
	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302, H332, H312, H319	<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

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## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

#### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

#### In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

#### In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

#### If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

### 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

### 5.2 Special hazards arising from the substance or mixture

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

### 5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

### 5.4 Further information

Use water spray to cool unopened containers.

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## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

## 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

## 6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

## 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### Advice on safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

#### Advice on protection against fire and explosion

Use explosion-proof equipment. **Advice on protection against fire and explosion**  
Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

#### Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.  
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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.  
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

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
Contains no substances with occupational exposure limit values.				
Acetonitrile-13C2	1722-25-4	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen Danger of cutaneous absorption		

		TWA	20 ppm 34 mg/m3	USA. NIOSH Recommended Exposure Limits
		TWA	40 ppm 70 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		STEL	60 ppm 105 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		TWA	40 ppm 70 mg/m3	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		PEL	40 ppm 70 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	60 ppm 105 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

Hazardous components without workplace control parameters

## 8.2 Exposure controls

### Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

### Personal protective equipment

#### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

#### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

#### Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

#### Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

#### Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## 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: -48 °C (-54 °F) - lit.
f) Initial boiling point and boiling range	81 - 82 °C 178 - 180 °F - lit.
g) Flash point	2.00 °C (35.60 °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: 16.00 %(V) Lower explosion limit: 4.40 %(V)
k) Vapor pressure	413.23 hPa at 55.00 °C (131.00 °F) 73.18 hPa at 15.00 °C(59.00 °F) 119.81 hPa at 25.00 °C(77.00 °F)
l) Vapor density	No data available
m) Density	0.824 g/mL at 25 °C (77 °F)0.824 g/cm <sup>3</sup> at 25 °C (77 °F)
Relative density	No data available
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	log Pow: -0.340
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

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

## 10.2 Chemical stability

Stable under recommended storage conditions.

## 10.3 Possibility of hazardous reactions

Vapors may form explosive mixture with air.

## 10.4 Conditions to avoid

Heat, flames and sparks.

## 10.5 Incompatible materials

acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

## 10.6 Hazardous decomposition products

No data available

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Mouse - male and female - 617 mg/kg

(OECD Test Guideline 401)

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

LC50 Inhalation - Mouse - male and female - 4 h - 6.022 mg/l

(OECD Test Guideline 403)

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

Acute toxicity estimate Dermal - 1,500 mg/kg

(Expert judgment)

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: Acetonitrile

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h

(OECD Test Guideline 404)

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

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

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

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

#### Respiratory or skin sensitization

Buehler Test - Guinea pig

Result: negative

(OECD Test Guideline 406)

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

#### Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Result: negative

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Remarks: (ECHA)

The value is given in analogy to the following substances: Acetonitrile  
Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Method: US-EPA

Result: negative

Remarks: The value is given in analogy to the following substances: Acetonitrile  
Test Type: Mutagenicity (mammal cell test); chromosome aberration.

Test system: Chinese hamster ovary cells

Metabolic activation: with and without metabolic activation

Result: Positive results were obtained in some in vitro tests.

Remarks: (National Toxicology Program)

The value is given in analogy to the following substances: Acetonitrile  
Test Type: sister chromatid exchange assay

Test system: Chinese hamster ovary cells

Metabolic activation: Metabolic activation

Result: negative

Remarks: The value is given in analogy to the following substances: Acetonitrile  
Test system: Saccharomyces cerevisiae

Metabolic activation: without metabolic activation

Result: positive

Remarks: Cytogenetic analysis

(ECHA)

The value is given in analogy to the following substances: Acetonitrile  
Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 476

Result: negative

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

Test Type: Micronucleus test

Species: Mouse

Application Route: Intraperitoneal

Method: OECD Test Guideline 474

Result: negative

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

### **Carcinogenicity**

No evidence of carcinogenicity in animal studies.

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**

Animal testing did not show any effects on fertility.

### **Specific target organ toxicity - single exposure**

The substance or mixture is not classified as specific target organ toxicant, single exposure.



**Specific target organ toxicity - repeated exposure**

The substance or mixture is not classified as specific target organ toxicant, repeated exposure. **Aspiration hazard**

No aspiration toxicity classification

**11.2 Additional Information**

Treat as cyanide poisoning., Always have on hand a cyanide first-aid kit, together with proper instructions., The onset of symptoms is generally delayed pending conversion to cyanide., Nausea, Vomiting, Diarrhea, Headache, Dizziness, Rash, Cyanosis, excitement, depression, Drowsiness, impaired judgment, Lack of coordination, stupor, death  
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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**SECTION 12: Ecological information****12.1 Toxicity**

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 1,640 mg/l - 96 h Remarks: (ECHA) The value is given in analogy to the following substances: Acetonitrile
Toxicity to algae	static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253) Remarks: The value is given in analogy to the following substances: Acetonitrile (Acetonitrile-13C2)  static test ErC50 - Phaeodactylum tricornutum - 9,696 mg/l - 72 h (ISO 10253) Remarks: The value is given in analogy to the following substances: Acetonitrile (Acetonitrile-13C2)
Toxicity to bacteria	Remarks: The value is given in analogy to the following substances: Acetonitrile (Acetonitrile-13C2)

**12.2 Persistence and degradability**

Biodegradability	Result: 70 % - Readily biodegradable. (OECD Test Guideline 310) Remarks: The value is given in analogy to the following substances: Acetonitrile
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**12.3 Bioaccumulative potential**

No bioaccumulation is to be expected ( $\log Pow \leq 4$ ).

**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 Other adverse effects

Avoid release to the environment.

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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

#### DOT (US)

UN number: 1648    Class: 3    Packing group: II  
Proper shipping name: Acetonitrile  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 1648    Class: 3    Packing group: II    EMS-No: F-E, S-D  
Proper shipping name: ACETONITRILE

#### IATA

UN number: 1648    Class: 3    Packing group: II  
Proper shipping name: Acetonitrile

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## SECTION 15: Regulatory information

#### SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

#### 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

#### Massachusetts Right To Know Components

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

#### Pennsylvania Right To Know Components

Acetonitrile-13C2	CAS-No. 1722-25-4	Revision Date 2007-07-01
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## New Jersey Right To Know Components

Acetonitrile-13C2

CAS-No.  
1722-25-4

Revision Date  
2007-07-01

## California Prop. 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

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## SECTION 16: Other information

### Further information

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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](http://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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