

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.2

Revision Date 08.09.2022

Print Date 02.05.2025

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name : Acetonitrile-d₃
Acetonitrile-d 3
Product Number : 569550
Brand : Aldrich
REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No. : 2206-26-0

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

Identified uses : Laboratory chemicals, Manufacture of substances

1.3

CHEMIKART

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Classification according to Regulation (EC) No 1272/2008

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 2), H319

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

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word	Danger
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, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P301 + P312	IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water.
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.
Supplemental Hazard Statements	none

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word	Danger
Hazard statement(s)	none
Precautionary statement(s)	none
Supplemental Hazard Statements	none

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.1 Substances

Synonyms	: Trideuteroacetone Methyl-d3 cyanide
Formula	: C ₂ D ₃ N
Molecular weight	: 44,07 g/mol
CAS-No.	: 2206-26-0
EC-No.	: 218-616-5

Component		Classification	Concentration
Acetonitrile deuteration			
CAS-No.	2206-26-0	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2; H225, H302, H332, H312, H319	<= 100 %
EC-No.	218-616-5		

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

Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. If breathing stops: mouth-to-mouth breathing or artificial respiration. Oxygen if necessary. Immediately call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: immediately make victim drink water (two glasses at most). 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

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Carbon dioxide (CO₂) Foam 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

Nitrogen oxides (NO_x)

Combustible.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

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. Suppress (knock down) gases/vapors/mists with a water spray jet. 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. Chemisorb®). 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 safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

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.

Handle and 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

8.2 Exposure controls

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). Safety glasses

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 EN374 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact

Material: Chloroprene

Minimum layer thickness: 0,65 mm

Break through time: 30 min

Material tested: KCL 720 Camapren®

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

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) Physical state | clear, liquid |
| b) Color | colorless |

- | | |
|---|--|
| c) Odor | pungent |
| d) Melting point/freezing point | No data available |
| e) Initial boiling point and boiling range | 80,7 °C - lit. |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 16 %(V)
Lower explosion limit: 3,0 %(V) |
| h) Flash point | 2,00 °C - closed cup |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: No data available |
| m) Water solubility | soluble |
| n) Partition coefficient: n-octanol/water | log Pow: -0,340 - Bioaccumulation is not expected. |
| o) Vapor pressure | 413,23 hPa at 55,00 °C
73,18 hPa at 15,00 °C
119,81 hPa at 25,00 °C |
| p) Density | 0,844 g/mL at 25 °C - lit. |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| s) Explosive properties | No data available |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

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

10.3 Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents
fuming sulfuric acid
conc. sulfuric acid
Strong bases
strong reducing agents
Generates dangerous gases or fumes in contact with:
acids
Risk of explosion with:
nitrates
perchlorates
perchloric acid
conc. sulfuric acid
with
Heat.
Risk of ignition or formation of inflammable gases or vapours with:
Oxidizing agents
Nitric acid
nitrogen dioxide
with
Catalyst

10.4 Conditions to avoid

Warming.

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 - Mouse - male and female - 617 mg/kg

(OECD Test Guideline 401)

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

Acute toxicity estimate Oral - 617 mg/kg

(Calculation method)

LC50 Inhalation - Mouse - male and female - 4 h - 6,022 mg/l - vapor

(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: 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

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

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: Sister chromatid exchange

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.

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

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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.

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 deuteration) 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 deuteration)
Toxicity to bacteria	Remarks: The value is given in analogy to the following substances:

Acetonitrile
(Acetonitrile deuteration)

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

12.3 Bioaccumulative potential

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

The value is given in analogy to the following substances:

12.4 Mobility in soil

Not expected to adsorb on soil.

12.5 Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Product:

Assessment

: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

12.7 Other adverse effects

Other adverse effects
Avoid release to the environment.

Stability in water

DT50 - > 9.999 d pH 7 at 25 °C

Remarks: (calculated)Hydrolyzes slowly.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1648

IMDG: 1648

IATA: 1648

14.2 UN proper shipping name

ADR/RID: ACETONITRILE

IMDG: ACETONITRILE

IATA: Acetonitrile

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances.

Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements referred to under sections 2 and 3.

H225	Highly flammable liquid and vapor.
H302	Harmful if swallowed.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H312	Harmful in contact with skin.
H319	Causes serious eye irritation.
H332	Harmful if inhaled.

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.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

Details in analogy to the undeuterated compound.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the

information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

CHEMIKART