

Safety Data Sheet

according to Regulation (EC) No 1907/2006 (REACH)
Classifications according to Regulation (EC) No 1272/2008.
Printdate 17 Oct 2025

1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product name:

Acetonitrile-d3

1.1. Catalog No.:

1001-1X50ML

1.2. Relevant identified uses of the substance or mixture

Identified: Laboratory chemical
uses: R&D

1.3. Uses advised against:

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2. HAZARDS IDENTIFICATION

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

2.2.1. Pictogram



2.2.2.

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.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms : Trideuteroacetonitrile

Methyl-d3 cyanide

Formula : C2D3N

Molecular weight : 44,07 g/mol

CAS-No. : 2206-26-0

EC-No. : 218-616-5

Component Acetonitrile deuteration CAS-No. : 2206-26-0

EC-No. : 218-616-5

Classification Flam. Liq. 2; Acute Tox. 4;

Eye Irrit. 2; H225, H302,

H332, H312, H319

Concentration <= 100 %

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

3.1.1. Formula

C2D3N

3.1.2. Molecular Weight (g/mol)

44.07

3.1.3. CAS-No.

2206-26-0

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

5. FIRE-FIGHTING 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.

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.

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.
hygroscopic Handle and store under inert gas.
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

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-30124 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.

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/cm³ 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

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

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: AcetonitrileTest 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: AcetonitrileTest 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: AcetonitrileTest 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: AcetonitrileTest system:

Saccharomyces cerevisiae

Metabolic activation: without metabolic activation

Result: positive

Remarks: Cytogenetic analysis
(ECHA)

The value is given in analogy to the following substances: AcetonitrileTest 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.

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

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.

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 <= 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:

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

Avoid release to the environment.

Stability in water DT50 - > 9.999 d pH 7 at 25 °C

Remarks: (calculated)Hydrolyzes slowly.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

No data available

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

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www.armar-europa.de

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.

: FLAMMABLE LIQUIDS

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

16. OTHER 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. For lab use only!