

Safety Data Sheet

Acetonitrile-d3

Classification acc. to 29 CFR 1910.1200

Version number: GHS 4.1
Replaces version of: 2025-06-10 (GHS 3)

Revision: 2025-06-12

SECTION 1: Identification

1.1 Product identifier

Identification of the substance	Acetonitrile-d3
CAS number	2206-26-0
Alternative name(s)	CD3CN

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

Relevant identified uses	general use
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1.3 Details of the supplier of the safety data sheet

Zeochem AG Joweid 5, CH-8630 Rüti Switzerland	Telephone: +41 44 922 93 93 e-Mail: info@zeochem.com Website: https://www.zeochem.com
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1.4 Emergency telephone number

Poison center		
Country	Name	Telephone
Switzerland	Toxzentrum Zürich / Tox. Info Suisse	+41 44 251 51 51 / CH: 145 - 24h/7d
United States	CHEMTREC USA	+1 800 424 9300 - 24h/7d

SECTION 2: Hazard(s) identification

2.1 Classification of the substance or mixture

Classification acc. to OSHA "Hazard Communication Standard" (29 CFR 1910.1200)

Section	Hazard class	Category	Hazard class and category	Hazard statement
A.1O	acute toxicity (oral)	4	Acute Tox. 4	H302
A.1D	acute toxicity (dermal)	4	Acute Tox. 4	H312
A.1I	acute toxicity (inhal.)	4	Acute Tox. 4	H332
A.3	serious eye damage/eye irritation	2	Eye Irrit. 2	H319
B.6	flammable liquid	2	Flam. Liq. 2	H225

For full text of abbreviations: see SECTION 16.

The most important adverse physicochemical, human health and environmental effects

The product is combustible and can be ignited by potential ignition sources.

2.2 Label elements

Labelling acc. to OSHA "Hazard Communication Standard" (29 CFR 1910.1200)

- Signal word danger

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2.2.1.2 Pictograms

GHS02, GHS07	 
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Hazard statements	
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 statements	
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
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	if swallowed: Call a poison center/doctor if you feel unwell
P302+P352	if on skin: Wash with plenty of water
P303+P361+P353	if on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/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
P312	call a poison center/doctor if you feel unwell
P321	specific treatment (see on this label)
P330	rinse mouth
P362+P364	take off contaminated clothing and wash it before reuse
P370+P378	in case of fire: Use sand, carbon dioxide or powder extinguisher 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

2.3 Other hazards

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Hazards not otherwise classified

May be harmful in contact with skin (GHS category 5: acutely toxic - dermal).

Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) in a concentration of $\geq 0.1\%$.

SECTION 3: Composition/information on ingredients

3.1 Substances

Name of substance	Acetonitrile-d3
Identifiers	
CAS No	2206-26-0
Molecular formula	C2D3N
Molar mass	44.1 g/mol

SECTION 4: First-aid measures

4.1 Description of first-aid measures

General notes

Do not leave affected person unattended. Remove victim out of the danger area. Keep affected person warm, still and covered. Take off immediately all contaminated clothing. In all cases of doubt, or when symptoms persist, seek medical advice. In case of unconsciousness place person in the recovery position. Never give anything by mouth.

Following inhalation

If breathing is irregular or stopped, immediately seek medical assistance and start first aid actions. Provide fresh air.

Following skin contact

Wash with plenty of soap and water.

Following eye contact

Remove contact lenses, if present and easy to do. Continue rinsing. Irrigate copiously with clean, fresh water for at least 10 minutes, holding the eyelids apart.

Following ingestion

Rinse mouth with water (only if the person is conscious). Do NOT induce vomiting.

4.2 Most important symptoms and effects, both acute and delayed

Symptoms and effects are not known to date.

4.3 Indication of any immediate medical attention and special treatment needed

none

SECTION 5: Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water spray, Alcohol resistant foam, BC-powder, Carbon dioxide (CO2)

Unsuitable extinguishing media

Water jet

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5.2 Special hazards arising from the substance or mixture

In case of insufficient ventilation and/or in use, may form flammable/explosive vapor-air mixture. Solvent vapors are heavier than air and may spread along floors. Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are particularly prone to the presence of flammable substances or mixtures.

Hazardous combustion products

Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO2)

5.3 Advice for firefighters

In case of fire and/or explosion do not breathe fumes. Coordinate firefighting measures to the fire surroundings. Do not allow firefighting water to enter drains or water courses. Collect contaminated firefighting water separately. Fight fire with normal precautions from a reasonable distance.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

For non-emergency personnel

Remove persons to safety.

For emergency responders

Wear breathing apparatus if exposed to vapors/dust/aerosols/gases.

6.2 Environmental precautions

Keep away from drains, surface and ground water. Retain contaminated washing water and dispose of it.

6.3 Methods and material for containment and cleaning up

Advice on how to contain a spill

Covering of drains

Advice on how to clean up a spill

Wipe up with absorbent material (e.g. cloth, fleece). Collect spillage: sawdust, kieselgur (diatomite), sand, universal binder

Appropriate containment techniques

Use of adsorbent materials.

Other information relating to spills and releases

Place in appropriate containers for disposal. Ventilate affected area.

6.4 Reference to other sections

Hazardous combustion products: see section 5. Personal protective equipment: see section 8. Incompatible materials: see section 10. Disposal considerations: see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Recommendations

Store in a dry place.

- Measures to prevent fire as well as aerosol and dust generation

Use local and general ventilation. Avoidance of ignition sources. Keep away from sources of ignition - No smoking. Take precautionary measures against static discharge. Use only in well-ventilated areas. Due to danger of explosion, prevent leakage of vapours into cellars, flues and ditches. Ground/bond container and receiving equipment. Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools.

- Specific notes/details

Places which are not ventilated, e.g. unventilated below ground level areas such as trenches, conduits and shafts, are

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particularly prone to the presence of flammable substances or mixtures. Vapors are heavier than air, spread along floors and form explosive mixtures with air. Vapors may form explosive mixtures with air.

Advice on general occupational hygiene

Wash hands after use. Do not eat, drink and smoke in work areas. Remove contaminated clothing and protective equipment before entering eating areas. Never keep food or drink in the vicinity of chemicals. Never place chemicals in containers that are normally used for food or drink. Keep away from food, drink and animal feedingstuffs.

7.2 Conditions for safe storage, including any incompatibilities

Managing of associated risks

- Explosive atmospheres

Keep container tightly closed and in a well-ventilated place. Use local and general ventilation. Keep cool. Protect from sunlight.

- Flammability hazards

Keep away from sources of ignition - No smoking. Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. Take precautionary measures against static discharge. Protect from sunlight.

- Ventilation requirements

Keep any substance that emits harmful vapors or gases in a place that allows these to be permanently extracted. Use local and general ventilation. Ground/bond container and receiving equipment.

- Specific designs for storage rooms or vessels

- Storage temperature

Recommended storage temperature: 18 – 22 °C
15 °C

- Packaging compatibilities

Only packagings which are approved (e.g. acc. to the Dangerous Goods Regulations) may be used.

7.3 Specific end use(s)

See section 16 for a general overview.

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Occupational exposure limit values (Workplace Exposure Limits)											
Country	Name of agent	CAS No	Identifier	TWA [ppm]	TWA [mg/m³]	STEL [ppm]	STEL [mg/m³]	Ceiling-C [ppm]	Ceiling-C [mg/m³]	Notation	Source
US	acetonitrile	75-05-8	REL	20 (10 h)	34 (10 h)						NIOSH REL
US	acetonitrile	75-05-8	PEL	40	70						29 CFR 1910.1000
US	acetonitrile	75-05-8	TLV®	20						H	ACGIH® 2023
US	acetonitrile (methyl cyanide)	75-05-8	PEL (CA)	40	70	60	105			H	Cal/OSHA PEL

Notation

Ceiling-C ceiling value is a limit value above which exposure should not occur

H absorbed through the skin

STEL short-term exposure limit: a limit value above which exposure should not occur and which is related to a 15-minute period (unless otherwise specified)

TWA time-weighted average (long-term exposure limit): measured or calculated in relation to a reference period of 8 hours

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Notation

time-weighted average (unless otherwise specified)

Environment values

Relevant PNECs and other threshold levels				
Endpoint	Threshold level	Organism	Environmental compartment	Exposure time
PNEC	10 mg/l	aquatic organisms	freshwater	short-term (single instance)
PNEC	1 mg/l	aquatic organisms	marine water	short-term (single instance)
PNEC	32 mg/l	aquatic organisms	sewage treatment plant (STP)	short-term (single instance)
PNEC	40.5 mg/kg	aquatic organisms	freshwater sediment	short-term (single instance)
PNEC	4.05 mg/kg	aquatic organisms	marine sediment	short-term (single instance)
PNEC	2.23 mg/kg	terrestrial organisms	soil	short-term (single instance)

8.2 Exposure controls

Appropriate engineering controls

General ventilation.

Individual protection measures (personal protective equipment)

Eye/face protection

Wear eye/face protection.

Skin protection

- Hand protection

Wear suitable gloves. Chemical protection gloves are suitable, which are tested according to EN 374. Check leak-tightness/impermeability prior to use. In the case of wanting to use the gloves again, clean them before taking off and air them well. For special purposes, it is recommended to check the resistance to chemicals of the protective gloves mentioned above together with the supplier of these gloves.

- Type of material

Nitrile

IIR: isobutene-isoprene (butyl) rubber

- Breakthrough times of the glove material

>30 minutes (permeation: level 2)

- Other protection measures

Take recovery periods for skin regeneration. Preventive skin protection (barrier creams/ointments) is recommended. Wash hands thoroughly after handling.

Respiratory protection

In case of inadequate ventilation wear respiratory protection.

Environmental exposure controls

Use appropriate container to avoid environmental contamination. Keep away from drains, surface and ground water.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Appearance

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Physical state	liquid
Color	colorless
Particle	not relevant (liquid)
Odor	characteristic

Other safety parameters

pH (value)	not determined
Melting point/freezing point	-45.7 °C at 101,325 Pa
Initial boiling point and boiling range	81.7 °C at 1,013 hPa
Flash point	2 °C (c.c.) (closed cup)
Evaporation rate	not determined
Flammability (solid, gas)	not relevant, (fluid)

Explosive limits

- Lower explosion limit (LEL)	3 vol%
- Upper explosion limit (UEL)	16 vol%
Vapor pressure	94.5 hPa at 20 °C
Density	0.84 g/cm³ at 20 °C
Vapor density	this information is not available

Solubility(ies)

- Water solubility	1,000,000 mg/l at 25 °C
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Partition coefficient

- n-octanol/water (log KOW)	-0.34 (pH value: ~7, 25 °C) (ECHA)
Auto-ignition temperature	524 °C at 101,325 Pa (ECHA)

Viscosity

- Kinematic viscosity	0.417 mm²/s at 20 °C
- Dynamic viscosity	0.35 mPa s at 20 °C
Explosive properties	none
Oxidizing properties	none

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9.2 Other information

Refractive index	1.34 (20 °C)
Temperature class (USA, acc. to NEC 500)	T1 (maximum permissible surface temperature on the equipment: 450°C)

SECTION 10: Stability and reactivity

10.1 Reactivity

Concerning incompatibility: see below "Conditions to avoid" and "Incompatible materials". It's a reactive substance. The mixture contains reactive substance(s). Risk of ignition.

If heated:

Risk of ignition

10.2 Chemical stability

See below "Conditions to avoid".

10.3 Possibility of hazardous reactions

No known hazardous reactions.

10.4 Conditions to avoid

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

Hints to prevent fire or explosion

Use explosion-proof electrical/ventilating/lighting/equipment. Use only non-sparking tools. Take precautionary measures against static discharge.

10.5 Incompatible materials

Oxidizers

10.6 Hazardous decomposition products

Reasonably anticipated hazardous decomposition products produced as a result of use, storage, spill and heating are not known. Hazardous combustion products: see section 5.

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Classification acc. to OSHA "Hazard Communication Standard" (29 CFR 1910.1200)

Acute toxicity

Harmful if swallowed. Harmful in contact with skin. Harmful if inhaled.

- Acute toxicity estimate (ATE)

Oral 469 mg/kg
Inhalation: vapor 11 mg/l/4h

Skin corrosion/irritation

Shall not be classified as corrosive/irritant to skin.

Serious eye damage/eye irritation

Causes serious eye irritation.

Respiratory or skin sensitization

Shall not be classified as a respiratory or skin sensitizer.

Germ cell mutagenicity

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Shall not be classified as germ cell mutagenic.

Carcinogenicity

Shall not be classified as carcinogenic.

Reproductive toxicity

Shall not be classified as a reproductive toxicant.

Specific target organ toxicity - single exposure

Shall not be classified as a specific target organ toxicant (single exposure).

Specific target organ toxicity - repeated exposure

Shall not be classified as a specific target organ toxicant (repeated exposure).

Aspiration hazard

Shall not be classified as presenting an aspiration hazard.

SECTION 12: Ecological information

12.1 Toxicity

Shall not be classified as hazardous to the aquatic environment.

12.2 Persistence and degradability

Biodegradation

The substance is readily biodegradable.

Process of degradability		
Process	Degradation rate	Time
carbon dioxide generation	70 %	21 d

12.3 Bioaccumulative potential

Data are not available.

n-octanol/water (log KOW)	-0.34 (pH value: ~7, 25 °C) (ECHA)
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12.4 Mobility in soil

Data are not available.

12.5 Results of PBT and vPvB assessment

According to the results of its assessment, this substance is not a PBT or a vPvB.

12.6 Endocrine disrupting properties

Does not contain an endocrine disruptor (ED) in a concentration of $\geq 0.1\%$.

12.7 Other adverse effects

Data are not available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Waste treatment-relevant information

Solvent reclamation/regeneration.

Sewage disposal-relevant information

Do not empty into drains. Avoid release to the environment. Refer to special instructions/safety data sheets.

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Waste treatment of containers/packages

Only packagings which are approved (e.g. acc. to DOT) may be used. Completely emptied packages can be recycled. Handle contaminated packages in the same way as the substance itself.

Remarks

Please consider the relevant national or regional provisions. Waste shall be separated into the categories that can be handled separately by the local or national waste management facilities.

SECTION 14: Transport information

14.1 UN number

DOT	UN 1648
IMDG-Code	UN 1648
ICAO-TI	UN 1648

14.2 UN proper shipping name

DOT	Acetonitrile
IMDG-Code	ACETONITRILE
ICAO-TI	Acetonitrile

14.3 Transport hazard class(es)

DOT	3
IMDG-Code	3
ICAO-TI	3

14.4 Packing group

DOT	II
IMDG-Code	II
ICAO-TI	II

14.5 Environmental hazards

non-environmentally hazardous acc. to the dangerous goods regulations

14.6 Special precautions for user

There is no additional information.

14.7 Transport in bulk according to IMO instruments

The cargo is not intended to be carried in bulk.

Information for each of the UN Model Regulations

Transport of dangerous goods by road or rail (49 CFR US DOT) - Additional information

Particulars in the shipper's declaration	UN1648, Acetonitrile, 3, II
Reportable quantity (RQ)	5,000 lbs (2,270 kg) (Acetonitrile-d3)
Danger label(s)	3



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Special provisions (SP) IB2, T7, TP2

ERG No 127

International Maritime Dangerous Goods Code (IMDG) - Additional information

Marine pollutant -

Danger label(s) 3



Excepted quantities (EQ) E2

Limited quantities (LQ) 1 L

EmS F-E, S-D

Stowage category B

International Civil Aviation Organization (ICAO-IATA/DGR) - Additional information

Danger label(s) 3



Excepted quantities (EQ) E2

Limited quantities (LQ) 1 L

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations specific for the product in question

National regulations (United States)

Toxic Substance Control Act (TSCA) substance is listed (ACTIVE)

Superfund Amendment and Reauthorization Act (SARA TITLE III)

- The List of Extremely Hazardous Substances and Their Threshold Planning Quantities (EPCRA Section 302, 304)

not listed

- Specific Toxic Chemical Listings (EPCRA Section 313)

Toxics Release Inventory: Specific Toxic Chemical Listings

Name of substance	CAS No	Remarks	Effective date
Acetonitrile-d3	75-05-8		1987-01-01

Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)

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- List of Hazardous Substances and Reportable Quantities (CERCLA section 102a) (40 CFR 302.4)

Name of substance	CAS No	Remarks	Statutory code	Final RQ pounds (Kg)
Acetonitrile-d3	75-05-8		3 4	5000 (2270)

Legend

3 "3" indicates that the source is section 112 of the Clean Air Act

4 "4" indicates that the source is section 3001 of the Resource Conservation and Recovery Act (RCRA)

Clean Air Act

not listed

Right to Know Hazardous Substance List

- Cleaning Product Right to Know Act Substance List (CA-RTK)

Name of substance	CAS No	Functionality	Authoritative Lists
Acetonitrile-d3	75-05-8		CA TACs OEHHHA RELs

- Toxic or Hazardous Substance List (MA-TURA)

Name of substance	CAS No	DEP CODE	PBT / HHS / LHS	PBT / HHS Threshold	De Minimis Concentration Threshold
Acetonitrile-d3	75-05-8				1.0 %

- Hazardous Substances List (MN-ERTK)

Name of substance	CAS No	References	Remarks
Acetonitrile-d3	75-05-8	A, N, O	skin

Legend

A American Conference of Governmental Industrial Hygienists (ACGIH), "Threshold Limit Values for Chemical Substances and Physical Agents and Biological Exposure Indices for 1992-93", available from ACGIH

N National Institute for Occupational Safety and Health (NIOSH), "Recommendations for Occupational Safety and Health Standards," August 1988, available from NIOSH, Publications Dissemination Office, Division of Standards Development and Technology Transfer

O Occupational Safety and Health Administration (OSHA), Safety and Health Standards, Code of Federal Regulations, title 29, part 1910, subpart Z, "Toxic and Hazardous Substances, 1990." General information: Minnesota Department of Labor and Industry, Occupational Safety and Health Division

skin If a potential for absorption from skin contact merits special consideration, the word "skin" follows the substance name.

- Hazardous Substance List (NJ-RTK)

Name of substance	CAS No	Remarks	Classifications
Acetonitrile-d3	75-05-8		F3

Legend

F3 Flammable - Third Degree

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- Hazardous Substance List (Chapter 323) (PA-RTK)

Name acc. to inventory	CAS No	Classification
ACETONITRILE	75-05-8	E

Legend

E Environmental hazard

- Hazardous Substance List (RI-RTK)

Name of substance	CAS No	References
Acetonitrile-d3	75-05-8	T, F

Legend

F Flammability (NFPA®)

T Toxicity (ACGIH®)

California Environmental Protection Agency (Cal/EPA): Proposition 65 - Safe Drinking Water and Toxic Enforcement Act of 1987

not listed

Industry or sector specific available guidance(s)

NPCA-HMIS® III

Hazardous Materials Identification System. American Coatings Association.

Category	Rating	Description
Chronic	/	none
Health	2	temporary or minor injury may occur
Flammability	3	material that can be ignited under almost all ambient temperature conditions
Physical hazard	0	material that is normally stable, even under fire conditions, and will not react with water, polymerize, decompose, condense, or self-react. Non-explosive
Personal protection	-	

NFPA® 704

National Fire Protection Association: Standard System for the Identification of the Hazards of Materials for Emergency Response (United States).

Category	Degree of hazard	Description
Flammability	3	material that can be ignited under almost all ambient temperature conditions
Health	2	material that, under emergency conditions, can cause temporary incapacitation or residual injury
Instability	0	material that is normally stable, even under fire conditions
Special hazard		

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National inventories

Country	Inventory	Status
EU	REACH Reg.	substance is listed
US	TSCA	substance is listed (ACTIVE)

Legend

REACH Reg. REACH registered substances
TSCA Toxic Substance Control Act

15.2 Chemical Safety Assessment

No Chemical Safety Assessment has been carried out for this substance.

SECTION 16: Other information, including date of preparation or last revision

Indication of changes (revised safety data sheet)

Section	Former entry (text/value)	Actual entry (text/value)	Safety-relevant
1.1		Alternative name(s): CD3CN	yes

Key literature references and sources for data

OSHA Hazard Communication Standard (HCS), 29 CFR 1910.1200.
Transport of dangerous goods by road or rail (49 CFR US DOT). International Maritime Dangerous Goods Code (IMDG). Dangerous Goods Regulations (DGR) for the air transport (IATA).

List of relevant phrases (code and full text as stated in section 2 and 3)

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

Disclaimer

This information is based upon the present state of our knowledge. This SDS has been compiled and is solely intended for this product.