

Chemical Safety Data Sheet MSDS / SDS

ACETONITRILE-D3

Revision Date:2025-10-04 Revision Number:1

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

Product identifier

Product name : ACETONITRILE-D3
CBnumber : CB6289320
CAS : 2206-26-0
EINECS Number : 218-616-5
Synonyms : CD3CN,Acetonitrile-d3

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.
Uses advised against : none

Company Identification

Company : Chemicalbook
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 010-86108875

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P403+P235 Store in a well-ventilated place. Keep cool.

Hazard statements

H225 Highly Flammable liquid and vapour

H302 Harmful if swallowed
H312 Harmful in contact with skin
H319 Causes serious eye irritation
H332 Harmful if inhaled

SECTION 3: Composition/information on ingredients

Substance

Product name	: ACETONITRILE-D3
Synonyms	: CD3CN, Acetonitrile-d3
CAS	: 2206-26-0
EC number	: 218-616-5
MF	: C2D3N
MW	: 44.07

SECTION 4: First aid measures

Description of first aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor

If inhaled

After inhalation: fresh air. Immediately call in physician. If breathing stops: immediately apply artificial respiration, if necessary also oxygen.

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.

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

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

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.

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. Risk of dust explosion.

Development of hazardous combustion gases or vapours possible in the event of fire. Forms explosive mixtures with air at ambient temperatures.

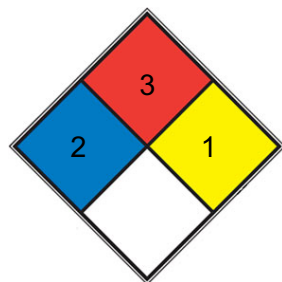
Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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.

NFPA 704



☒ HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

☒ FIRE 3 Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions . Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

☒ REACT 1 Normally stable, but can become unstable at elevated temperatures and pressures (e.g. [propene](#))

☐ SPEC.

☐ HAZ.

SECTION 6: Accidental release measures

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.

Environmental precautions

Do not let product enter drains. Risk of explosion.

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 carefully with liquid-absorbent material (e.g.

Chemisorb?). Dispose of properly. Clean up affected area.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

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.

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. Keep locked up or in an area accessible only to qualified or authorized persons.

hygroscopic Handle and store under inert gas.

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

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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

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.

Recommended Filter type: Filter type ABEK

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

Information on basic physicochemical properties

Appearance	colorless clear, liquid
Odour	pungent
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	-46 °C
Initial boiling point and boiling range	80,7 °C - lit.
Flash point	2,00 °C - closed cup
Evaporation rate	No data available
Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	Upper explosion limit: 16 %(V) Lower explosion limit: 3,0 %(V)
Vapour pressure	413,23 hPa at 55,00 °C 73,18 hPa at 15,00 °C 119,81 hPa at 25,00 °C

Vapour density	No data available
Relative density	0.844
Water solubility	soluble
Partition coefficient: n-octanol/water	log Pow: -0,340 - Bioaccumulation is not expected.
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

Vapors may form explosive mixture with air.

Chemical stability

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

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

Conditions to avoid

Warming.

Incompatible materials

rubber, various plastics

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Mouse - male and female - 617 mg/kg (OECD Test Guideline 401)

LC50 Inhalation - Mouse - male and female - 4 h - 6,022 mg/l (OECD Test Guideline 403)

Acute toxicity estimate Dermal - 1.500 mg/kg (Expert judgment)

Acute toxicity estimate Dermal - 1.500 mg/kg (Expert judgment)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation. (OECD Test Guideline 405)

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)

Germ cell mutagenicity

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation Result: negative

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

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)

Test Type: sister chromatid exchange assay Test system: Chinese hamster ovary cells Metabolic activation: Metabolic activation Result: negative

Remarks: Sister chromatid exchange Test system: Saccharomyces cerevisiae

Metabolic activation: without metabolic activation Result: positive

Remarks: Cytogenetic analysis (ECHA)

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

Test Type: Micronucleus test Species: Mouse

Application Route: Intraperitoneal Method: OECD Test Guideline 474 Result: negative

Carcinogenicity

No data available

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.

No aspiration toxicity classification

Toxicity

LD50 orally in Rabbit: 2730 - 3800 mg/kg LD50 dermal Rabbit 988 mg/kg

SECTION 12: Ecological information

Toxicity

Toxicity to fish

flow-through test LC50 - Pimephales promelas (fathead minnow) - 1.640 mg/l - 96 h

Remarks: (ECHA)

Toxicity to algae

static test NOEC - Phaeodactylum tricornutum - 400 mg/l - 72 h (ISO 10253)

static test ErC50 - Phaeodactylum tricornutum - 9.696 mg/l - 72 h (ISO 10253)

Toxicity to bacteria

Persistence and degradability

Biodegradability Result: 70 % - Readily biodegradable.

(OECD Test Guideline 310)

Bioaccumulative potential

No bioaccumulation is to be expected ($\log P_{ow} \leq 4$).

Mobility in soil

Not expected to adsorb on soil.

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.

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

Waste treatment methods

Product

SECTION 14: Transport information

UN number

ADR/RID: 1648 IMDG: 1648 IATA: 1648

UN proper shipping name

ADR/RID: ACETONITRILE IMDG: ACETONITRILE IATA: Acetonitrile

Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA: 3

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: no IMDG Marine pollutant: no IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

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

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

EC Inventory:Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

Vietnam National Chemical Inventory:Not Listed. website: <https://chemicaldata.gov.vn/>

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:
http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

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