

SAFETY DATA SHEET

Version 6.14
Revision Date 15.03.2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Acetonitrile

Product Number : 271004
Brand : Sigma-Aldrich
CAS-No. : 75-05-8

1.2 Other means of identification

Methyl cyanide
ACN

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

Identified uses : For R&D use only. Not for pharmaceutical, household or other uses.

1.4 Details of the supplier of the safety data sheet

Company : Merck Life Science Pty Ltd
Ground Floor, Building 1, 885 Mountain Highway
BAYSWATER VIC 3153
AUSTRALIA

Telephone : +61 1800 800 097
E-mail address : customersupport.anz@merckgroup.com

1.5 Emergency telephone

Emergency Phone # : Free call (24/7): 1800 862 115
Int'l (24/7): +61 2 9037 2994
(CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Inhalation (Category 4), H332
Acute toxicity, Dermal (Category 4), H312
Serious eye damage/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

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

Prevention

P210

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

P233

Keep container tightly closed.

P261

Avoid breathing mist or vapors.

P264

Wash skin thoroughly after handling.

P280

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

Response

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.

P337 + P313

If eye irritation persists: Get medical advice/ attention.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage

P403 + P235

Store in a well-ventilated place. Keep cool.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

Synonyms : Methyl cyanide
ACN

Formula : C₂H₃N

Molecular weight : 41.05 g/mol

CAS-No. : 75-05-8

EC-No. : 200-835-2

Index-No. : 608-001-00-3

Hazardous ingredients

Component	Classification	Concentration
Acetonitrile		
	Flam. Liq. 2; Acute Tox. 4;	<= 100 %

	Eye Dam./Irrit. 2A; H225, H302, H332, H312, H319	
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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

Water Foam Carbon dioxide (CO₂) 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)

Carbon oxides

Nitrogen oxides (NO_x)

Combustible.

Fire may cause evolution of:

nitrogen oxides, Hydrogen cyanide (hydrocyanic acid)

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. Chemizorb®). 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

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

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.3 no other specific uses are stipulated.

SECTION 8: Exposure controls/personal protection**8.1 Control parameters****Ingredients with workplace control parameters**

Component	CAS-No.	Value	Control parameters	Basis
Acetonitrile	75-05-8	TWA	40 ppm 67 mg/m ³	Australia. Workplace Exposure Standards for Airborne Contaminants.
	Remarks	Skin absorption		
		STEL	60 ppm 101 mg/m ³	Australia. Workplace Exposure Standards for Airborne Contaminants.
		Skin absorption		

Derived No Effect Level (DNEL)

Application Area	Routes of exposure	Health effect	Value
Workers	Inhalation	Acute local effects, Acute systemic effects	68 mg/m ³
Workers	Skin contact	Long-term systemic effects	32.2mg/kg BW/d
Workers	Inhalation	Long-term local effects, Long-term systemic effects	68 mg/m ³
Consumers	Inhalation	Acute local effects	220 mg/m ³
Consumers	Inhalation	Acute systemic effects	22 mg/m ³
Consumers	Inhalation	Long-term systemic effects	4.8 mg/m ³

Predicted No Effect Concentration (PNEC)

Compartment	Value
Water	10 mg/l
Soil	2.41 mg/kg
Sea water	1 mg/l
Fresh water	10 mg/l
Fresh water sediment	7.53 mg/kg
Onsite sewage treatment plant	32 mg/l

8.2 Exposure controls**Appropriate engineering controls**

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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 EN 16523-1 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 EN 16523-1 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: 10 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.

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 | ether-like |
| d) Melting point/freezing point | Melting point/range: -48 °C |
| e) Initial boiling point | 81 - 82 °C |

	and boiling range	
f)	Flammability (solid, gas)	No data available
g)	Upper/lower flammability or explosive limits	Upper explosion limit: 16 %(V) Lower explosion limit: 4.4 %(V)
h)	Flash point	2.0 °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: 0.350 Pas at 20.00 °C
m)	Water solubility	1,000 g/l at 25 °C completely soluble
n)	Partition coefficient: n-octanol/water	log Pow: -0.54 at 25 °C - Bioaccumulation is not expected.
o)	Vapor pressure	98.64 hPa at 20 °C
p)	Density	0.786 g/mL at 25 °C
	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

Surface tension	29.0 mN/m at 20.0 °C
Relative vapor density	1.42 - (Air = 1.0)

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:

Sigma-Aldrich- 271004

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Strong bases
strong reducing agents
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
Generates dangerous gases or fumes in contact with:
Acids

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)

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

(OECD Test Guideline 403)

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)

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)

Remarks: 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
Remarks: (ECHA)
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 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

RTECS: AL7700000

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)

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

Toxicity to fish(Chronic toxicity) flow-through test NOEC - Oryzias latipes - 102 mg/l - 21 d (OECD Test Guideline 204)

12.2 Persistence and degradability

Biodegradability Result: 70 % - Readily biodegradable. (OECD Test Guideline 310)

12.3 Bioaccumulative potential

No bioaccumulation is to be expected (log Pow <= 4).

12.4 Mobility in soil

Not expected to adsorb on soil.

12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

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.

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1648 IMDG: 1648 IATA-DGR: 1648

14.2 UN proper shipping name

ADR/RID: ACETONITRILE
IMDG: ACETONITRILE
IATA-DGR: Acetonitrile

14.3 Transport hazard class(es)

ADR/RID: 3 IMDG: 3 IATA-DGR: 3

14.4 Packaging group

ADR/RID: II IMDG: II IATA-DGR: II

14.5 Environmental hazards

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

14.6 Special precautions for user

None

14.7 Incompatible materials

Other regulations

Hazchem Code : •2YE

SECTION 15: Regulatory information

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

Therapeutic Goods (Poisons Standard) : No poison schedule number
Instrument allocated

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

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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.

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