SAFETY DATA SHEET

Version 8.7
Revision Date 02.07.2024
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SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

Product name : Acetonitrile for DNA synthesis (<= 30 ppm H2O)

Product Number : 1.13212
Catalogue No. : 113212
Brand : Millipore
CAS-No. : 75-05-8

1.2 Other means of identification

No data available

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

Identified uses : Reagent for analysis, Chemical production

1.4 Details of the supplier of the safety data sheet

Company : Merck Life Science Ltd
Level 26 PwC Tower, 15 Customs Street West
1010 AUCKLAND
NEW ZEALAND

Telephone : 0800 936 666
E-mail address : customersupport.anz@merckgroup.com

1.5 Emergency telephone

Emergency Phone # : 0800 0800 425 459 (CHEMTREC NZ)
+64 9 801 0034 (Int'l CHEMTREC)

SECTION 2: Hazards identification

2.1 GHS Classification

Flammable liquids (Category 2), H225
Acute toxicity, Oral (Category 2), H300
Acute toxicity, Inhalation (Category 3), H331
Acute toxicity, Dermal (Category 3), H311
Serious eye damage/eye irritation (Category 2), 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

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Signal Word	Danger

Hazard Statements

H225	Highly flammable liquid and vapor.
H300	Fatal if swallowed.
H311 + H331	Toxic 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.
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.

Response

P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

Storage

P403 + P233	Store in a well-ventilated place. Keep container tightly closed.

2.3 Other hazards - none

SECTION 3: Composition/information on ingredients

Substance / Mixture : Substance

3.1 Substances

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. 2; Acute Tox. 3; Eye Dam./Irrit. 2; H225, H300, H331, H311, H319	<= 100 %

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

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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 (NOx)
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.

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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
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.

Recommended storage temperature see product label.

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

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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	WES-TWA	40 ppm 67 mg/m3	New Zealand. Workplace Exposure Standards for Atmospheric Contaminants
	Remarks	Skin absorption		
		WES-STEL	60 ppm 101 mg/m3	New Zealand. Workplace Exposure Standards for Atmospheric Contaminants
		Skin absorption		

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.

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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	liquid
b)	Color	colorless
c)	Odor	ether-like
d)	Melting point/freezing point	Melting point/ range: -45.7 °C at 1,013 hPa
e)	Initial boiling point and boiling range	81.0 - 82.0 °C at 1,013.25 hPa
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	524.0 °C
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	0.78 g/cm3 at 20 °C
	Relative density	No data available
q)	Relative vapor density	No data available
r)	Particle characteristics	No data available

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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:
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
rubber, various plastics, Strong oxidizing agents

10.6 Hazardous decomposition products
In the event of fire: see section 5

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SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity
Acute toxicity estimate Oral - 5.1 mg/kg
(Expert judgment)
Acute toxicity estimate Inhalation - 4 h - 3.1 mg/l - vapor

(Expert judgment)
Acute toxicity estimate Dermal - 300.1 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)
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

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(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

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	

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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

Biological effects:
Hazard for drinking water supplies.
Discharge into the environment must be avoided.
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

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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
rubber, various plastics, Strong oxidizing agents

Other regulations
Hazchem Code : •2YE

SECTION 15: Regulatory information

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

National regulatory information
HSNO Approval Code: HSR001071

HSNO Group Standard Approval: not required
Tracking Required: not required
Approved Handler Cert.: not required

SECTION 16: Other information

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

H225	Highly flammable liquid and vapor.
H300	Fatal if swallowed.
H311	Toxic in contact with skin.
H319	Causes serious eye irritation.
H331	Toxic 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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