SAFETY DATA SHEET

Version 6.16
Revision Date 31.12.2025
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Section 1: Identification

1.1 Product identifiers

Product name : Acetonitrile hypergrade for LC-MS Li-Chrosolv®

Product Number : 1.00029
Catalogue No. : 100029
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

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 number

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

Section 2: Hazard identification

GHS Classification

Eye irritation : Category A

Flammable liquids : Category 2

Acute toxicity (Oral) : Category 2

Acute toxicity (Inhalation) : Category 3

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Acute toxicity (Dermal) : Category 3

Serious eye damage/eye irritation : Category 2

GHS label elements

Hazard pictograms :

Signal word : Danger

Hazard statements : H225 Highly flammable liquid and vapour.
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.

Other hazards which do not result in classification

None known.

Section 3: Composition/information on ingredients

Substance / Mixture : Substance

CAS-No. : 75-05-8

Components

Chemical name	CAS-No.	Concentration (% w/w)
Acetonitrile	75-05-8	>= 90 -<= 100

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Section 4: First-aid measures

General advice	:	Show this 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.
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
Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

Section 5: Fire-fighting measures

Suitable extinguishing media	:	Water Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Fire may cause evolution of: nitrogen oxides Hydrogen cyanide (hydrocyanic acid)

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Pay attention to flashback.

Vapours 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.

Hazardous combustion products	:	Carbon oxides Nitrogen oxides (NOx)
Specific extinguishing methods	:	Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	:	Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.
Hazchem Code	:	2YE

Section 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapours, 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. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	:	Do not let product enter drains. Risk of explosion.

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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.

Section 7: Handling and storage

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	:	Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.
Further information on storage conditions	:	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.
Storage class	:	3, Flammable liquids
Recommended storage temperature	:	Recommended storage temperature see product label.
Further information on storage stability	:	Recommended storage temperature see product label.

Section 8: Exposure controls/personal protection

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
Acetonitrile	75-05-8	WES-TWA	10 ppm 17 mg/m3	NZ OEL
	Further information: Skin absorption			
		WES-STEL	20 ppm 34 mg/m3	NZ OEL
	Further information: Skin absorption			
		TWA	20 ppm	ACGIH

Engineering measures : No data available

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Personal protective equipment

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 A (acc. to DIN 3181) for vapours of organic compounds

The entrepeneur 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.

Hand protection

Material	:	butyl-rubber
Break through time	:	480 min
Glove thickness	:	0.7 mm
Protective index	:	Full contact
Manufacturer	:	Butoject® (KCL 898)
Material	:	Chloroprene
Break through time	:	10 min
Glove thickness	:	0.65 mm
Protective index	:	Splash contact
Manufacturer	:	KCL 720 Camapren®
Remarks	:	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).

Eye protection	:	Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses
Skin and body protection	:	Flame retardant antistatic protective clothing.

Section 9: Physical and chemical properties

Appearance	:	liquid (20 °C , 1,013 hPa)

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Color	:	colourless
Odor	:	ether-like
Odor Threshold	:	39.8 ppm
pH	:	No data available
Melting point/ range	:	-45.7 °C (1,013 hPa)
Boiling point/boiling range	:	81.0 - 82.0 °C (1,013.25 hPa)
Flash point	:	2.0 °C Method: closed cup
Evaporation rate	:	5.8
Flammability (solid, gas)	:	No data available
Flammability (liquids)	:	No data available
Burning rate	:	No data available
Upper explosion limit / Upper flammability limit	:	Upper flammability limit 16 %(V)
Lower explosion limit / Lower flammability limit	:	Lower flammability limit 4.4 %(V)
Vapor pressure	:	98.64 hPa (20 °C)
Relative vapour density	:	1.42 (Air = 1.0)
Relative density	:	No data available
Density	:	0.78 g/cm3 (20 °C)
Solubility(ies) Water solubility	:	1,000 g/l (25 °C) completely soluble
Partition coefficient: n-octanol/water	:	log Pow: -0.54 (25 °C) Bioaccumulation is not expected.

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Autoignition temperature	:	523 °C (1,013 hPa)
Decomposition temperature	:	No data available
Viscosity		
Viscosity, dynamic	:	0.350 Pas (20.00 °C)
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Surface tension	:	29.0 mN/m, 20.0 °C
Refractive index	:	1.344 (20 °C)
Molecular weight	:	41.05 g/mol
Particle characteristics		
Particle size	:	No data available

Section 10: Stability and reactivity

Reactivity	:	Vapours 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: 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

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Conditions to avoid	:	Warming.
Incompatible materials	:	rubber various plastics
Hazardous decomposition products	:	In the event of fire: see section 5

Section 11: Toxicological information

11.1 Information on toxicological effects

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

(Expert judgement)
Acute toxicity estimate Dermal - 300.1 mg/kg
(Expert judgement)

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

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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

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, Diarrhoea, 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.

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Section 12: Ecological information

Ecotoxicity

Components:

Acetonitrile:

Toxicity to fish	:	LC50 (Pimephales promelas (fathead minnow)): 1,640 mg/l Exposure time: 96 h Test Type: flow-through test Analytical monitoring: yes Remarks: (ECHA)
Toxicity to algae/aquatic plants	:	NOEC (Phaeodactylum tricornutum): 400 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: ISO 10253 GLP: yes ErC50 (Phaeodactylum tricornutum): 9,696 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: ISO 10253 GLP: yes
Toxicity to fish (Chronic toxicity)	:	NOEC (Oryzias latipes): 102 mg/l End point: mortality Exposure time: 21 d Test Type: flow-through test Analytical monitoring: yes Method: OECD Test Guideline 204 GLP: yes
Toxicity to microorganisms	:	EC50 (activated sludge): > 1,000 mg/l Exposure time: 30 min Test Type: static test Method: OECD Test Guideline 209 GLP: yes

Persistence and degradability

Components:

Acetonitrile:

Biodegradability	:	Inoculum: activated sludge, non-adapted Concentration: 684 mg/l Result: Readily biodegradable. Biodegradation: 70 % Exposure time: 21 d

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Method: OECD Test Guideline 310
GLP: yes

Stability in water : Degradation half life (DT50): > 9,999 d pH: 7
Hydrolysis: at 25 °C
Remarks: (calculated)
Hydrolyses slowly.

Bioaccumulative potential

Components:

Acetonitrile:

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

Partition coefficient: n-octanol/water : log Pow: -0.54 (25 °C)
Remarks: Bioaccumulation is not expected.

Mobility in soil

Components:

Acetonitrile:

Distribution among environmental compartments : Adsorption/Soil
Koc: 16, log Koc: 1.21
Remarks: Mobile in soils
(Lit.)

Stability in soil : Dissipation time: > 168 - < 672 h
Method: (calculated)
Remarks: Not expected to adsorb on soil.

Other adverse effects

Product:

Additional ecological information : Biological effects:

Hazard for drinking water supplies.

Discharge into the environment must be avoided.

Components:

Acetonitrile:

Additional ecological information : Avoid release to the environment.

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Section 13: Disposal considerations

Disposal methods

Waste from residues	:	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

International Regulations

IATA-DGR

UN/ID No.	:	UN 1648
Proper shipping name	:	Acetonitrile
Class	:	3
Packing group	:	II
Labels	:	Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	364
Packing instruction (passenger aircraft)	:	353

IMDG-Code

UN number	:	UN 1648
Proper shipping name	:	ACETONITRILE
Class	:	3
Packing group	:	II
Labels	:	3
EmS Code	:	F-E, S-D
Marine pollutant	:	no

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

National Regulations

NZS 5433

UN number	:	UN 1648
Proper shipping name	:	ACETONITRILE
Class	:	3
Packing group	:	II
Labels	:	3
Hazchem Code	:	2YE
Marine pollutant	:	no

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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Section 15: Regulatory information

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

HSNO Approval Number

HSR001071 Acetonitrile

Tolerable Exposure Limits (TEL)

Not applicable

Environmental Exposure Limits (EEL)

Not applicable

HSW Controls

Certified handler certificate required.
Tracking hazardous substance is required.
Refer to the Health and Safety at Work (Hazardous Substances) Regulations 2017, for further information.

Section 16: Other information

Revision Date	:	31.12.2025

Further information

Other 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. Copyright 2025 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.
Date format	:	dd.mm.yyyy

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NZ OEL	:	New Zealand. Workplace Exposure Standards for Atmospheric Contaminants
ACGIH / TWA	:	8-hour, time-weighted average
NZ OEL / WES-TWA	:	Workplace Exposure Standard - Time Weighted aver-

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		age
NZ OEL / WES-STEL	:	Workplace Exposure Standard - Short-Term Exposure Limit

AIIC - Australian Inventory of Industrial Chemicals; ANTT - National Agency for Transport by Land of Brazil; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MERCOSUR - The Agreement for the Facilitation of the Transport of Dangerous Goods; n.o.s. - Not Otherwise Specified; Nch - Chilean Norm; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NOM - Official Mexican Norm; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TDG - Transportation of Dangerous Goods; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative; WHMIS - Workplace Hazardous Materials Information System

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