

# SAFETY DATA SHEET

Version 6.11  
Revision Date 01.03.2023  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Acetonitrile hypergrade for LC-MS  
LiChrosolv®

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 : Sigma-Aldrich Pte Ltd  
(Co. Registration No. 199403788W)  
2 Science Park Drive  
#05-01/12 Ascent Building  
SINGAPORE 118222  
SINGAPORE

Telephone : +65 6890 6633  
Fax : +65 6890 6639  
E-mail address : TechnicalService@merckgroup.com

### 1.5 Emergency telephone

Emergency Phone # : 1-800-262-8200

## 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 statement(s)	
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 statement(s)	
Prevention	
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P233	Keep container tightly closed.
P261	Avoid breathing mist or vapors.
P264	Wash skin thoroughly after handling.
P280	Wear protective gloves/ eye protection/ face protection.
Response	
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
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.

**Reduced Labeling (<= 125 ml)**

Pictogram



Signal Word	none
Hazard statement(s)	none
Precautionary statement(s)	none

Refer to the Safety Data Sheet before use.

**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
<b>Acetonitrile</b>	Flam. Liq. 2; Acute Tox. 4; Eye Dam./Irrit. 2A; H225, H302, H332, H312, H319	<= 100 %

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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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) 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<sub>x</sub>)

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.

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## 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. Chemisorb®). Dispose of properly. Clean up affected area.

### 6.4 Reference to other sections

For disposal see section 13.

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## 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 1.3 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

Millipore- 1.00029

Page 4 of 11

The life science business of Merck operates as MilliporeSigma in the US and Canada



Component	CAS-No.	Value	Control parameters	Basis
Acetonitrile	75-05-8	PEL (long term)	40 ppm 67 mg/m <sup>3</sup>	Singapore. Workplace Safety and Health Act - First Schedule Permissible Exposure Limits of Toxic Substances
		PEL (short term)	60 ppm 101 mg/m <sup>3</sup>	Singapore. Workplace Safety and Health Act - First Schedule Permissible Exposure Limits of Toxic Substances

## 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 EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://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](http://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.

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## 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)<br>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<br>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/cm <sup>3</sup> at 20 °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)   |

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## **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

### **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**

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**

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.

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**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**

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.

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## 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.

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## 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

rubber, various plastics

#### Other regulations

Hazchem Code                      : •2YE

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## SECTION 15: Regulatory information

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

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## 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 above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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](http://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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