

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 7.6

Revision Date 29.04.2023

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

## 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  
Index-No. : 608-001-00-3  
REACH No. : 01-2119471307-38-XXXX  
CAS-No. : 75-05-8

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

Identified uses : Reagent for analysis

### 1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Chemie GmbH  
Eschenstrasse 5  
D-82024 TAUFKIRCHEN

Telephone : +49 (0)89 6513-1130  
Fax : +49 (0)89 6513-1161  
E-mail address : technischerservice@merckgroup.com

### 1.4 Emergency telephone

Emergency Phone # : 0800 181 7059 (CHEMTREC Deutschland)  
+49 (0)696 43508409 (CHEMTREC  
weltweit)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### Classification according to Regulation (EC) No 1272/2008

Flammable liquids (Category 2), H225  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Inhalation (Category 4), H332  
Acute toxicity, Dermal (Category 4), H312  
Eye irritation (Category 2), H319

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

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## 2.2 Label elements

### Labelling according Regulation (EC) No 1272/2008

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)

P210

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

P280

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

P301 + P312

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.

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.

P305 + P351 + P338

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard Statements

none

### Reduced Labeling (<= 125 ml)

Pictogram



Signal Word

Danger

Hazard statement(s)

none

Precautionary statement(s)

none

Supplemental Hazard Statements

none

## 2.3 Other hazards

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.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Formula

: C<sub>2</sub>H<sub>3</sub>N

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Molecular weight : 41,05 g/mol  
 CAS-No. : 75-05-8  
 EC-No. : 200-835-2  
 Index-No. : 608-001-00-3

Component	Classification	Concentration
<b>Acetonitrile</b>		
CAS-No. 75-05-8 EC-No. 200-835-2 Index-No. 608-001-00-3	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2; H225, H302, H332, H312, 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

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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 1.2 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

##### Derived No Effect Level (DNEL)

Application Area	Routes of exposure	Health effect	Value
Worker DNEL, acute	inhalation	Systemic effects	68 mg/m <sup>3</sup>
Worker DNEL, acute	inhalation	Local effects	68 mg/m <sup>3</sup>
Worker DNEL, longterm	dermal	Systemic effects	
Worker DNEL, longterm	inhalation	Systemic effects	68 mg/m <sup>3</sup>
Worker DNEL, longterm	inhalation	Local effects	68 mg/m <sup>3</sup>

##### Predicted No Effect Concentration (PNEC)

Compartment	Value
Fresh water	10 mg/l
Sea water	1 mg/l
Aquatic intermittent release	10 mg/l
Sewage treatment plant	32 mg/l
Soil	3,02 mg/kg
Fresh water sediment	45 mg/kg
Sea sediment	4,5 mg/kg

### 8.2 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](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**

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

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.

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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) 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/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

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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)

Acute toxicity estimate Oral - 617 mg/kg

(Calculation method)

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

### Endocrine disrupting properties

#### Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

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.

### 12.6 Endocrine disrupting properties

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**Product:**

Assessment

: The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

**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**

No data available

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**SECTION 14: Transport information****14.1 UN number**

ADR/RID: 1648

IMDG: 1648

IATA: 1648

**14.2 UN proper shipping name**

ADR/RID: ACETONITRILE

IMDG: ACETONITRILE

IATA: Acetonitrile

**14.3 Transport hazard class(es)**

ADR/RID: 3

IMDG: 3

IATA: 3

**14.4 Packaging group**

ADR/RID: II

IMDG: II

IATA: II

**14.5 Environmental hazards**

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

**14.6 Special precautions for user**

Tunnel restriction code : (D/E)

Further information : No data available

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**SECTION 15: Regulatory information****15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

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## Authorisations and/or restrictions on use

### National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances. P5c FLAMMABLE LIQUIDS

### Other regulations

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

## 15.2 Chemical Safety Assessment

A Chemical Safety Assessment has been carried out for this substance.

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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.
H302 + H312 + H332	Harmful if swallowed, in contact with skin or if inhaled.
H312	Highly flammable liquid and vapor.
H319	Harmful if swallowed, in contact with skin or if inhaled.
H332	Causes serious eye irritation.



## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; 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; GHS - Globally Harmonized 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; 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

## 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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