

# SAFETY DATA SHEET

Version 6.21  
Revision Date 09/08/2024  
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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  
Index-No. : 608-001-00-3  
CAS-No. : 75-05-8

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

Identified uses : Laboratory chemicals, Synthesis of substances  
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

#### GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

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 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

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242

Use only non-sparking tools.

P243

Take precautionary measures against static discharge.

P261

Avoid breathing mist or vapors.

P264

Wash skin thoroughly after handling.

P270

Do not eat, drink or smoke when using this product.

P271

Use only outdoors or in a well-ventilated area.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P312 + P330

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

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.

P305 + P351 + P338

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

P337 + P313

If eye irritation persists: Get medical advice/ attention.

P363

Wash contaminated clothing before reuse.

P370 + P378

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

P403 + P235

Store in a well-ventilated place. Keep cool.

P501

Dispose of contents/ container to an approved waste disposal plant.

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Synonyms : Methyl cyanide

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## ACN

Formula	: C <sub>2</sub> H <sub>3</sub> N
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>		
	Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; 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>)

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**

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 1.2 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	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen Danger of cutaneous absorption		
		TWA	20 ppm 34 mg/m <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
		TWA	40 ppm 70 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		PEL	40 ppm 70 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		
		STEL	60 ppm 105 mg/m <sup>3</sup>	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

### Derived No Effect Level (DNEL)

Application Area	Routes of exposure	Health effect	Value
Workers	Inhalation	Acute local effects, Acute systemic effects	68 mg/m <sup>3</sup>
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 <sup>3</sup>
Consumers	Inhalation	Acute local effects	220 mg/m <sup>3</sup>
Consumers	Inhalation	Acute systemic effects	22 mg/m <sup>3</sup>
Consumers	Inhalation	Long-term systemic effects	4.8 mg/m <sup>3</sup>

### 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](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 EN 16523-1 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.

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) Appearance                                   | Form: clear, liquid<br>Color: colorless                           |
| b) Odor   | ether-like  |
| c) Odor Threshold                               | 39.8 ppm  |
| d) pH   | No data available   |
| e) Melting point/freezing point                 | Melting point/ range: -48 °C (-54 °F)                             |
| f) Initial boiling point and boiling range      | 81 - 82 °C 178 - 180 °F   |
| g) Flash point                                  | 2.0 °C (35.6 °F) - closed cup                                     |
| h) Evaporation rate                             | 5.8   |
| i) Flammability (solid, gas)                    | No data available   |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 16 %(V)<br>Lower explosion limit: 4.4 %(V) |
| k) Vapor pressure                               | 98.64 hPa at 20 °C (68 °F)  |
| l) Vapor density                                | 1.42 - (Air = 1.0)  |
| m) Density                                      | 0.786 g/mL at 25 °C (77 °F)                                       |
| Relative density                                | No data available   |
| n) Water solubility                             | 1,000 g/l at 25 °C (77 °F)completely soluble                      |
| o) Partition coefficient:                       | log Pow: -0.54 at 25 °C (77 °F) - Bioaccumulation is not          |

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n-octanol/water	expected.
p) Autoignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	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 (68.0 °F)
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

No data available

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## 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

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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.

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **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.

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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)
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### 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.
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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****DOT (US)**

UN number: 1648 Class: 3 Packing group: II  
Proper shipping name: Acetonitrile  
Reportable Quantity (RQ): 5000 lbs  
Poison Inhalation Hazard: No

**IMDG**

UN number: 1648 Class: 3 Packing group: II EMS-No: F-E, S-D  
Proper shipping name: ACETONITRILE

**IATA**

UN number: 1648 Class: 3 Packing group: II  
Proper shipping name: Acetonitrile

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**SECTION 15: Regulatory information****CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Acetonitrile	75-05-8	5000	5000

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard

**SARA 313** : The following components are subject to reporting levels established by SARA Title III, Section 313:  
Acetonitrile 75-05-8 >= 90 - <= 100 %

**Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

Acetonitrile 75-05-8 >= 90 - <= 100 %

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

Acetonitrile 75-05-8 >= 90 - <= 100 %

### Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### US State Regulations

#### Massachusetts Right To Know

Acetonitrile 75-05-8

#### Pennsylvania Right To Know

Acetonitrile 75-05-8

#### Maine Chemicals of High Concern

Product does not contain any listed chemicals

#### Vermont Chemicals of High Concern

Product does not contain any listed chemicals

#### Washington Chemicals of High Concern

Product does not contain any listed chemicals

### The ingredients of this product are reported in the following inventories:

TSCA : All substances listed as active on the TSCA inventory

### TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## SECTION 16: Other information

### 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](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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