

1. PRODUCT AND COMPANY IDENTIFICATION

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

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich
3050 Spruce Street
SAINT LOUIS MO 63103
USA

Telephone : +1 800-325-5832

Fax : +1 800-325-5052

1.4 Emergency telephone number

Emergency Phone # : +1-703-527-3887 (CHEMTREC)

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 statement(s)

H225 Highly flammable liquid and vapour.
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/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 dust/ fume/ gas/ mist/ vapours/ spray. |
| 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

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

| | | |
|---------------------|---|---------------------------------|
| Synonyms | : | Methyl cyanide ACN |
| Formula | : | C ₂ H ₃ N |
| Molecular weight | : | 41.05 g/mol |
| CAS-No. | : | 75-05-8 |
| EC-No. | : | 200-835-2 |
| Index-No. | : | 608-001-00-3 |
| Registration number | : | 01-2119471307-38-XXXX |

Hazardous components

| Component | Classification | Concentration |
|---------------------|---------------------------------------------------------------------------|---------------|
| Acetonitrile | Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302 + H312 + H332, H319 | 90 - 100 % |

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

4. FIRST AID MEASURES

4.1 Description of first aid measures

General advice

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

5. FIREFIGHTING MEASURES**5.1 Extinguishing media****Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

5.2 Special hazards arising from the substance or mixture

No data available

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

6. ACCIDENTAL RELEASE MEASURES**6.1 Personal precautions, protective equipment and emergency procedures**

Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13).

6.4 Reference to other sections

For disposal see section 13.

7. HANDLING AND STORAGE**7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Use explosion-proof equipment. Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Handle and store under inert gas.

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSONAL PROTECTION**8.1 Control parameters****Components with workplace control parameters**

| Component | CAS-No. | Value | Control parameters | Basis |
|--------------|---------|----------------------------------------------------------------------------------------------------------------|----------------------------------|-----------------------------------------------------------------------------------------|
| Acetonitrile | 75-05-8 | TWA | 20.000000 ppm | USA. ACGIH Threshold Limit Values (TLV) |
| | Remarks | Lower Respiratory Tract irritation Not classifiable as a human carcinogen Danger of cutaneous absorption | | |
| | | TWA | 20.000000 ppm 34.000000 mg/m3 | USA. NIOSH Recommended Exposure Limits |
| | | Forms cyanide in the body. | | |
| | | TWA | 40.000000 ppm 70.000000 mg/m3 | USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants |
| | | The value in mg/m3 is approximate. | | |
| | | PEL | 40 ppm 70 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |
| | | STEL | 60 ppm 105 mg/m3 | California permissible exposure limits for chemical contaminants (Title 8, Article 107) |
| | | Skin | | |

Derived No Effect Level (DNEL)

| Application Area | Exposure routes | Health effect | Value |
|------------------|-----------------|-----------------------------------------------------|----------------|
| Workers | Inhalation | Acute local effects, Acute systemic effects | 68 mg/m3 |
| Workers | Skin contact | Long-term systemic effects | 32.2mg/kg BW/d |
| Workers | Inhalation | Long-term local effects, Long-term systemic effects | 68 mg/m3 |
| Consumers | Inhalation | Acute local effects | 220 mg/m3 |
| Consumers | Inhalation | Acute systemic effects | 22 mg/m3 |
| Consumers | Inhalation | Long-term systemic effects | 4.8 mg/m3 |

Predicted No Effect Concentration (PNEC)

| Compartment | Value |
|-------------------------------|------------|
| Water | 10 mg/l |
| Soil | 2.41 mg/kg |
| Marine 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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

Splash contact
Material: butyl-rubber
Minimum layer thickness: 0.3 mm
Break through time: 480 min
Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

- | | |
|-------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| a) Appearance | Form: clear, liquid Colour: colourless |
| b) Odour | ether-like |
| c) Odour Threshold | No data available |
| 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) Lower explosion limit: 3 %(V) |
| k) Vapour pressure | 73.18 hPa (54.89 mmHg) at 15 °C (59 °F) 121.44 hPa (91.09 mmHg) at 25 °C (77 °F) 413.23 hPa (309.95 mmHg) at 55 °C (131 °F) 98.64 hPa (73.99 mmHg) at 20 °C (68 °F) |
| l) Vapour density | 1.42 - (Air = 1.0) |
| m) Relative density | 0.786 g/mL at 25 °C (77 °F) |
| n) Water solubility | completely soluble |

- o) Partition coefficient: n-octanol/water log Pow: -0.54 at 25 °C (77 °F)
- p) Auto-ignition temperature 524.0 °C (975.2 °F)
- q) Decomposition temperature No data available
- r) Viscosity No data available
- s) Explosive properties Not explosive
- t) Oxidizing properties The substance or mixture is not classified as oxidizing.

9.2 Other safety information

- Surface tension 29.0 mN/m at 20.0 °C (68.0 °F)
- Relative vapour density 1.42 - (Air = 1.0)

10. STABILITY AND REACTIVITY

10.1 Reactivity

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

Vapours may form explosive mixture with air.

10.4 Conditions to avoid

Heat, flames and sparks. Extremes of temperature and direct sunlight.

10.5 Incompatible materials

acids, Bases, Oxidizing agents, Reducing agents, Alkali metals

10.6 Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NOx)

In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 1,320 - 6,690 mg/kg

LC50 Inhalation - Mouse - 4 h - 3587 ppm
(OECD Test Guideline 403)

LC50 Inhalation - Rat - 4 h - 26.8 mg/l

LD50 Dermal - Rabbit - male and female - > 2,000 mg/kg
(OECD Test Guideline 402)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation
(OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irritating to eyes.
(OECD Test Guideline 405)

Respiratory or skin sensitisation

Buehler Test - Guinea pig

Did not cause sensitisation on laboratory animals.
(OECD Test Guideline 406)

Germ cell mutagenicity

Hamster

ovary

Result: negative

Mutation in mammalian somatic cells.

Ames test

S. typhimurium

Result: Not mutagenic in Ames Test

Hamster

ovary

Result: Equivocal evidence.

Sister chromatid exchange

Mutagenicity (micronucleus test)

Mouse

Result: Positive results were obtained in some in vivo tests.

Carcinogenicity

No evidence of carcinogenicity in animal studies.

IARC: No component 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 component 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 identified as a carcinogen or potential carcinogen by OSHA.

Reproductive toxicity

No data available

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

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, 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.

12. ECOLOGICAL INFORMATION

12.1 Toxicity

Toxicity to fish LC50 - *Pimephales promelas* (fathead minnow) - 1,640.00 mg/l - 96 h

NOEC - *Oryzias latipes* - 102 mg/l - 21 d

Toxicity to daphnia and other aquatic invertebrates EC50 - *Daphnia magna* (Water flea) - 3,600 mg/l - 48 h
(OECD Test Guideline 202)

NOEC - *Daphnia magna* (Water flea) - 160 mg/l - 21 d

12.2 Persistence and degradability

Biodegradability Result: 84 % - Readily biodegradable.
(OECD Test Guideline 301C)

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 Other adverse effects

Avoid release to the environment.

Stability in water

Remarks: Hydrolyses slowly.

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods

Product

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

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

15. REGULATORY INFORMATION

SARA 302 Components

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

SARA 313 Components

The following components are subject to reporting levels established by SARA Title III, Section 313:

| | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01 |

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components

| | CAS-No. | Revision Date |
|--------------|---------|---------------|
| Acetonitrile | 75-05-8 | 2007-07-01 |

Pennsylvania Right To Know Components

| | CAS-No. | Revision Date |
|--|---------|---------------|
|--|---------|---------------|

Acetonitrile

75-05-8

2007-07-01

New Jersey Right To Know Components

Acetonitrile

CAS-No.
75-05-8

Revision Date
2007-07-01

California Prop. 65 Components

This product does not contain any chemicals known to State of California to cause cancer, birth defects, or any other reproductive harm.

16. OTHER INFORMATION

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

| | |
|-----------------------|-----------------------------------------------------------|
| Acute Tox. | Acute toxicity |
| Eye Irrit. | Eye irritation |
| Flam. Liq. | Flammable liquids |
| H225 | Highly flammable liquid and vapour. |
| H302 | Harmful if swallowed. |
| H302 + H312 + H332 | Harmful if swallowed, in contact with skin or if inhaled. |
| H312 | Harmful in contact with skin. |

HMIS Rating

| | |
|------------------------|---|
| Health hazard: | 2 |
| Chronic Health Hazard: | |
| Flammability: | 3 |
| Physical Hazard | 0 |

NFPA Rating

| | |
|--------------------|---|
| Health hazard: | 2 |
| Fire Hazard: | 3 |
| Reactivity Hazard: | 0 |
| Health hazard: | 2 |
| Fire Hazard: | 3 |
| Reactivity Hazard: | 0 |

Further information

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Preparation Information

Sigma-Aldrich Corporation
Product Safety – Americas Region
1-800-521-8956

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