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.
P336  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  
| Formula              | C₂H₃N  
| 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

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitrile</td>
<td>Flam. Liq. 2; Acute Tox. 4; Eye Irrit. 2A; H225, H302 + H312 + H332, H319 &lt;= 100 %</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitrile</td>
<td>75-05-8</td>
<td>TWA</td>
<td>20.000000 ppm</td>
<td>USA, ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

Remarks: Lower Respiratory Tract irritation
Not classifiable as a human carcinogen
Danger of cutaneous absorption

<table>
<thead>
<tr>
<th>TWA</th>
<th>20.000000 ppm 34.000000 mg/m³</th>
<th>USA, NIOSH Recommended Exposure Limits</th>
</tr>
</thead>
</table>

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.

### Derived No Effect Level (DNEL)

<table>
<thead>
<tr>
<th>Application Area</th>
<th>Exposure routes</th>
<th>Health effect</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Workers</td>
<td>Inhalation</td>
<td>Acute local effects, Acute systemic effects</td>
<td>68 mg/m³</td>
</tr>
<tr>
<td>Workers</td>
<td>Skin contact</td>
<td>Long-term systemic effects</td>
<td>32.2 mg/kg BW/d</td>
</tr>
<tr>
<td>Workers</td>
<td>Inhalation</td>
<td>Long-term local effects, Long-term systemic effects</td>
<td>68 mg/m³</td>
</tr>
<tr>
<td>Consumers</td>
<td>Inhalation</td>
<td>Acute local effects</td>
<td>220 mg/m³</td>
</tr>
<tr>
<td>Consumers</td>
<td>Inhalation</td>
<td>Acute systemic effects</td>
<td>22 mg/m³</td>
</tr>
<tr>
<td>Consumers</td>
<td>Inhalation</td>
<td>Long-term systemic effects</td>
<td>4.8 mg/m³</td>
</tr>
</tbody>
</table>

### Predicted No Effect Concentration (PNEC)

<table>
<thead>
<tr>
<th>Compartment</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>10 mg/l</td>
</tr>
<tr>
<td>Soil</td>
<td>2.41 mg/kg</td>
</tr>
<tr>
<td>Marine water</td>
<td>1 mg/l</td>
</tr>
<tr>
<td>Fresh water</td>
<td>10 mg/l</td>
</tr>
<tr>
<td>Fresh water sediment</td>
<td>7.53 mg/kg</td>
</tr>
<tr>
<td>Onsite sewage treatment plant</td>
<td>32 mg/l</td>
</tr>
</tbody>
</table>

#### 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

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:

<table>
<thead>
<tr>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitrile</td>
<td>75-05-8</td>
</tr>
</tbody>
</table>

SARA 311/312 Hazards
Fire Hazard, Acute Health Hazard

Massachusetts Right To Know Components
Acetonitrile
CAS-No. 75-05-8 Revision Date 2007-07-01

Pennsylvania Right To Know Components
Acetonitrile
CAS-No. 75-05-8 Revision Date 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 + Harmful if swallowed, in contact with skin or if inhaled
H332         Harmful in contact with skin.

HMIS Rating
Health hazard: 2
Chronic Health Hazard: 0
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

Version: 4.8                  Revision Date: 03/08/2016                  Print Date: 05/16/2017