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

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
The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

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

SECTION 3: Composition/information on ingredients

3.1 Substances
Synonyms : Methyl cyanide
            ACN
Formula : C₂H₃N
Molecular weight : 41.05 g/mol
CAS-No. : 75-05-8
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

SECTION 5: Firefighting measures

5.1 Extinguishing media

**Suitable extinguishing media**
Water Foam Carbon dioxide (CO2) 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 (NOx)
Carbon oxides
Nitrogen oxides (NOx)
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.

**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. Chemizorb®). Dispose of properly. Clean up affected area.

6.4 **Reference to other sections**
For disposal see section 13.

**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

### SECTION 8: Exposure controls/personal protection

#### 8.1 Control parameters

**Ingredients with workplace 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 ppm</td>
<td>USA. ACGIH Threshold Limit Values (TLV)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Not classifiable as a human carcinogen</td>
</tr>
<tr>
<td>Danger of cutaneous absorption</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 ppm</td>
<td>TWA</td>
<td>USA. NIOSH Recommended Exposure Limits</td>
</tr>
<tr>
<td>40 ppm</td>
<td>TWA</td>
<td>USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants</td>
</tr>
<tr>
<td>40 ppm</td>
<td>PEL</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>60 ppm</td>
<td>STEL</td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Value</th>
<th>Control parameters</th>
<th>Basis</th>
</tr>
</thead>
<tbody>
<tr>
<td>68 mg/m3</td>
<td></td>
<td>California permissible exposure limits for chemical contaminants (Title 8, Article 107)</td>
</tr>
</tbody>
</table>

#### Derived No Effect Level (DNEL)

<table>
<thead>
<tr>
<th>Application Area</th>
<th>Routes of exposure</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>
</tbody>
</table>

Sigma-Aldrich - 271004
<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Workers</strong></td>
<td><strong>Skin contact</strong></td>
<td><strong>Long-term systemic effects</strong></td>
<td><strong>32.2mg/kg BW/d</strong></td>
</tr>
<tr>
<td><strong>Workers</strong></td>
<td><strong>Inhalation</strong></td>
<td><strong>Long-term local effects, Long-term systemic effects</strong></td>
<td><strong>68 mg/m³</strong></td>
</tr>
<tr>
<td><strong>Consumers</strong></td>
<td><strong>Inhalation</strong></td>
<td>Acute local effects</td>
<td><strong>220 mg/m³</strong></td>
</tr>
<tr>
<td><strong>Consumers</strong></td>
<td><strong>Inhalation</strong></td>
<td>Acute systemic effects</td>
<td><strong>22 mg/m³</strong></td>
</tr>
<tr>
<td><strong>Consumers</strong></td>
<td><strong>Inhalation</strong></td>
<td>Long-term systemic effects</td>
<td><strong>4.8 mg/m³</strong></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>Sea 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**
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).

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).

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.

SECTION 9: Physical and chemical properties
9.1 Information on basic physical and chemical properties

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

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)

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

10.6 Hazardous decomposition products
In the event of fire: see section 5
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.

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.

SECTION 12: Ecological information

12.1 Toxicity
Toxicity to fish flow-through test LC50 - Pimephales promelas (fathead minnow) -
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
Avoid release to the environment.
Stability in water DT50 - > 9,999 d pH 7 at 25 °C
Remarks: (calculated) Hydrolyzes slowly.

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.

SECTION 14: Transport information

DOT (US)
UN number: 1648 Class: 3 Packing group: II
Sigma-Aldrich - 271004
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

---

**SECTION 15: Regulatory information**

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

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

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitrile</td>
<td>75-05-8</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

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

**Massachusetts Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitrile</td>
<td>75-05-8</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>

**Pennsylvania Right To Know Components**

<table>
<thead>
<tr>
<th>Component</th>
<th>CAS-No.</th>
<th>Revision Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetonitrile</td>
<td>75-05-8</td>
<td>2007-07-01</td>
</tr>
</tbody>
</table>
SECTION 16: Other information

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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Version: 6.17 Revision Date: 11/22/2023 Print Date: 12/09/2023