1. PRODUCT AND COMPANY IDENTIFICATION

1.1 Product identifiers

Product name: Benzonitrile
Product Number: B8959
Brand: Sigma-Aldrich
Index-No.: 608-012-00-3
CAS-No.: 100-47-0

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

Identified uses: Laboratory chemicals, Manufacture 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 #: (314) 776-6555

2. HAZARDS IDENTIFICATION

2.1 Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)
Flammable liquids (Category 4), H227
Acute toxicity, Oral (Category 4), H302
Acute toxicity, Dermal (Category 4), H312
Skin irritation (Category 2), H315
Acute aquatic toxicity (Category 3), H402

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: Warning

Hazard statement(s)
H227 Combustible liquid.
H302 + H312 Harmful if swallowed or in contact with skin
H315 Causes skin irritation.
H402 Harmful to aquatic life.

Precautionary statement(s)
P210 Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
2.3 Hazards not otherwise classified (HNOC) or not covered by GHS

Vesicant.

3. COMPOSITION/INFORMATION ON INGREDIENTS

3.1 Substances

Synonyms: Phenyl cyanide

Formula: C₇H₅N

Molecular weight: 103.12 g/mol

CAS-No.: 100-47-0

EC-No.: 202-855-7

Index-No.: 608-012-00-3

<table>
<thead>
<tr>
<th>Component</th>
<th>Classification</th>
<th>Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzonitrile</td>
<td>Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Aquatic Acute 3; H227, H302 + H312, H315, H402</td>
<td>&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
Flush eyes with water as a precaution.

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
Carbon oxides, Nitrogen oxides (NOx)

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. 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. Discharge into the environment must be avoided.

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). Keep in suitable, closed containers for disposal.

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. 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. hygroscopic Handle and store under inert gas. Storage class (TRGS 510): Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

7.3 Specific end use(s)
Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

8. EXPOSURE CONTROLS/PERSOAL PROTECTION

8.1 Control parameters
Components with workplace control parameters
Contains no substances with occupational exposure limit values.

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, 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 multipurpose 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. Discharge into the environment must be avoided.

9. PHYSICAL AND CHEMICAL PROPERTIES

9.1 Information on basic physical and chemical properties

a) Appearance  
Form: liquid  
Colour: colourless

b) Odour  
No data available

c) Odour Threshold  
No data available

d) pH  
No data available

e) Melting point/freezing point  
Melting point/range: -13 °C (9 °F) - lit.

f) Initial boiling point and boiling range  
191 °C (376 °F) - lit.

g) Flash point  
70 °C (158 °F) - closed cup

h) Evaporation rate  
No data available

i) Flammability (solid, gas)  
No data available

j) Upper/lower flammability or explosive limits  
Upper explosion limit: 7.2 %(V)  
Lower explosion limit: 1.4 %(V)

k) Vapour pressure  
1 hPa (1 mmHg) at 20 °C (68 °F)

l) Vapour density  
3.56 - (Air = 1.0)
m) Relative density 1.000 g/cm³
n) Water solubility ca. 10 g/l
o) Partition coefficient: n-octanol/water log Pow: 1.56
p) Auto-ignition temperature No data available
q) Decomposition temperature No data available
r) Viscosity No data available
s) Explosive properties No data available
t) Oxidizing properties No data available

9.2 Other safety information
- Surface tension 38.79 mN/m at 25 °C (77 °F)
- Relative vapour density 3.56 - (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
No data available

10.4 Conditions to avoid
Heat, flames and sparks.

10.5 Incompatible materials
Strong bases, Strong oxidizing agents, Strong reducing agents, acids, Chlorates, Nitrates, Plastics

10.6 Hazardous decomposition products
Other decomposition products - No data available
In the event of fire: see section 5

11. TOXICOLOGICAL INFORMATION
11.1 Information on toxicological effects

Acute toxicity
LD50 Oral - Mouse - 971 mg/kg
LC50 Inhalation - Mouse - 1,800 mg/m³
LD50 Dermal - Rabbit - 1,250 mg/kg
No data available

Skin corrosion/irritation
Skin - Rabbit
Result: Moderate skin irritation - 24 h

Serious eye damage/eye irritation
No data available

Respiratory or skin sensitisation
No data available

Germ cell mutagenicity
No data available

Carcinogenicity
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.

ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

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

Specific target organ toxicity - single exposure
No data available

Specific target organ toxicity - repeated exposure
No data available

Aspiration hazard
No data available

Additional Information
RTECS: DI2450000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.
Stomach - Irregularities - Based on Human Evidence
Stomach - Irregularities - Based on Human Evidence

12. ECOLOGICAL INFORMATION

12.1 Toxicity
Toxicity to fish LC50 - Oncorhynchus mykiss (rainbow trout) - 32 mg/l - 96 h

12.2 Persistence and degradability
Biodegradability Biotic/Aerobic
Result: - Readily biodegradable.
Biotic/Aerobic - Exposure time 7 d

12.3 Bioaccumulative potential
No data available

12.4 Mobility in soil
No data available

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
An environmental hazard cannot be excluded in the event of unprofessional handling or disposal. Harmful to aquatic life.
No data available

13. DISPOSAL CONSIDERATIONS

13.1 Waste treatment methods
Product
This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Offer surplus and non-recyclable solutions to a licensed disposal company.

Contaminated packaging
Dispose of as unused product.
14. TRANSPORT INFORMATION

**DOT (US)**
- UN number: 2224
- Class: 6.1
- Packing group: II
- Proper shipping name: Benzonitrile
- Reportable Quantity (RQ): 5000 lbs
- Poison Inhalation Hazard: No

**IMDG**
- UN number: 2224
- Class: 6.1
- Packing group: II
- EMS-No: F-A, S-A
- Proper shipping name: BENZONITRILE

**IATA**
- UN number: 2224
- Class: 6.1
- Packing group: II
- Proper shipping name: Benzonitrile

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**
This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**
- Fire Hazard
- Acute Health Hazard
- Chronic Health Hazard

**Massachusetts Right To Know Components**
- Benzonitrile
  - CAS-No.: 100-47-0
  - Revision Date: 1993-04-24

**Pennsylvania Right To Know Components**
- Benzonitrile
  - CAS-No.: 100-47-0
  - Revision Date: 1993-04-24

**New Jersey Right To Know Components**
- Benzonitrile
  - CAS-No.: 100-47-0
  - Revision Date: 1993-04-24

**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
- **Aquatic Acute** Acute aquatic toxicity
- **Flam. Liq.** Flammable liquids
- **H227** Combustible liquid.
- **H302** Harmful if swallowed.
- **H302 + H312** Harmful if swallowed or in contact with skin
- **H312** Harmful in contact with skin.

**HMIS Rating**
- Health hazard: 1
- Chronic Health Hazard: *
- Flammability: 2
- Physical Hazard: 0
NFPA Rating
Health hazard: 1
Fire Hazard: 2
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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