

## SAFETY DATA SHEET

Version 4.4  
Revision Date 12/01/2014  
Print Date 06/02/2015

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**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

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**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.

P280	Wear protective gloves/ eye protection/ face protection.
P301 + P312 + P330	IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell. Rinse mouth.
P302 + P352	IF ON SKIN: Wash with plenty of soap and water.
P302 + P352 + P312	IF ON SKIN: Wash with plenty of soap and water. Call a POISON CENTER or doctor/ physician if you feel unwell.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash before reuse.
P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
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

Vesicant.

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

Synonyms	: Phenyl cyanide
Formula	: C <sub>7</sub> H <sub>5</sub> N
Molecular weight	: 103.12 g/mol
CAS-No.	: 100-47-0
EC-No.	: 202-855-7
Index-No.	: 608-012-00-3

#### Hazardous components

Component	Classification	Concentration
<b>Benzonitrile</b>		
	Flam. Liq. 4; Acute Tox. 4; Skin Irrit. 2; Aquatic Acute 3; H227, H302 + H312, H315, H402	<= 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

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

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## 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 (NO<sub>x</sub>)

### 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.

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## 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.

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## 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

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## 8. EXPOSURE CONTROLS/PERSONAL 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 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. Discharge into the environment must be avoided.

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## **9. PHYSICAL AND CHEMICAL PROPERTIES**

### **9.1 Information on basic physical and chemical properties**

- |   |  |
|---|--|
| a) Appearance                                   | Form: liquid<br>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)<br>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/cm <sup>3</sup>
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)

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## 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

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Mouse - 971 mg/kg

LC50 Inhalation - Mouse - 1,800 mg/m<sup>3</sup>

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

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

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**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

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**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.

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## 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

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## 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

	CAS-No.	Revision Date
Benzonitrile	100-47-0	1993-04-24

### Pennsylvania Right To Know Components

	CAS-No.	Revision Date
Benzonitrile	100-47-0	1993-04-24

### New Jersey Right To Know Components

	CAS-No.	Revision Date
Benzonitrile	100-47-0	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.

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## 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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