

# SAFETY DATA SHEET

Version 6.7  
Revision Date 03/07/2024  
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## SECTION 1: Identification of the substance/mixture and of the company/undertaking

### 1.1 Product identifiers

Product name : Benzonitrile

Product Number : 294098

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, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

### 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

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## 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 4), H227  
Acute toxicity, Oral (Category 4), H302  
Acute toxicity, Dermal (Category 4), H312

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 Statements

H227

H302 + H312

Combustible liquid.

Harmful if swallowed or in contact with skin.

Precautionary Statements

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.

P280

Wear protective gloves/ eye protection/ face protection.

P301 + P312 + P330

IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.

P302 + P352 + P312

IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.

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

Vesicant.

## SECTION 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

Component	Classification	Concentration
<b>benzonitrile</b>		
	Flam. Liq. 4; Acute Tox. 4; H227, H302, H312	<= 100 %

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

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## 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.

#### **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. 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

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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 (NO<sub>x</sub>)

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 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.

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## 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.

### 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.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

#### 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

Tightly closed. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

hygroscopic Handle and store under inert gas.

#### Storage class

Storage class (TRGS 510): 6.1A: 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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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

### 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](http://www.kcl.de)).

Full contact

Material: Viton®

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

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](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 30 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

##### Body Protection

protective clothing

##### Respiratory protection

Recommended Filter type: Filter type ABEK

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.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

a) Appearance	Form: liquid Color: colorless
b) Odor	No data available
c) Odor 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) Vapor pressure	1 hPa at 20 °C (68 °F) 133 hPa at 123.5 °C(254.3 °F)
l) Vapor density	3.56 - (Air = 1.0)
m) Density	1.000 g/cm <sup>3</sup>
Relative density	1.005
n) Water solubility	0.001 g/l at 25 °C (77 °F) - slightly soluble
o) Partition coefficient: n-octanol/water	log Pow: 1.5 at 20 °C (68 °F) - Bioaccumulation is not expected.
p) Autoignition temperature	ca.615 °C (ca.1139 °F) at 1,013 hPa
q) Decomposition temperature	No data available
r) Viscosity	1.054 mm <sup>2</sup> /s at 37.78 °C (100.00 °F) -
s) Explosive properties	No data available
t) Oxidizing properties	none

### 9.2 Other safety information

Surface tension 0.03 mN/m at 25 °C (77 °F)

Relative vapor 3.56 - (Air = 1.0)

Sigma-Aldrich - 294098

Page 6 of 11

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

**Millipore**  
**Sigma**

density

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## **SECTION 10: Stability and reactivity**

### **10.1 Reactivity**

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### **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 oxidizing agents

acids

### **10.4 Conditions to avoid**

Avoid moisture. Do not heat over: 30°C

Strong heating.

### **10.5 Incompatible materials**

No data available

### **10.6 Hazardous decomposition products**

In the event of fire: see section 5

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## **SECTION 11: Toxicological information**

### **11.1 Information on toxicological effects**

#### **Acute toxicity**

LD50 Oral - Rat - male and female - 1,000 mg/kg  
(OECD Test Guideline 401)

Symptoms: Nausea, Vomiting

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - 1,400 mg/kg

Remarks: (ECHA)

#### **Skin corrosion/irritation**

Skin - Rabbit

Result: Mild skin irritation - 24 h

Remarks: (ECHA)

Remarks: Possible damages:

slight irritation

#### **Serious eye damage/eye irritation**

Eyes - Rabbit

Result: No eye irritation

Remarks: (ECHA)

### **Respiratory or skin sensitization**

Patch test: - Human

Result: negative

Remarks: (IUCLID)

### **Germ cell mutagenicity**

Test Type: Ames test

Test system: S. typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

### **Carcinogenicity**

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**

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

## **11.2 Additional Information**

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

After absorption:

Vertigo  
Headache  
Drowsiness  
confusion  
Impairment of vision  
drop in blood pressure  
respiratory paralysis  
Coma  
Unconsciousness  
Convulsions

The following applies to cyanogen compounds/ nitriles in general: utmost caution! Release of hydrocyanic acid is possible - blockade of cellular respiration. Cardiovascular disorders, dyspnoea, unconsciousness.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## **SECTION 12: Ecological information**

### **12.1 Toxicity**

Toxicity to fish	LC50 - Oncorhynchus mykiss (rainbow trout) - 32 mg/l - 96 h Remarks: (External MSDS)
Toxicity to algae	Cell multiplication inhibition test IC50 - Chlorella vulgaris (Fresh water algae) - 231 mg/l - 6 h Remarks: (IUCLID) (benzonitrile)
Toxicity to bacteria	Remarks: (IUCLID) (benzonitrile)

### **12.2 Persistence and degradability**

Biodegradability	aerobic - Exposure time 14 d Result: 100 % - Readily biodegradable. (OECD Test Guideline 301E)
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### **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 Endocrine disrupting properties**

No data available

### **12.7 Other adverse effects**

No data available

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## **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.

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## **SECTION 14: Transport information**

#### **DOT (US)**

UN number: 2224 Class: 6.1  
Proper shipping name: Benzonitrile  
Reportable Quantity (RQ): 5000 lbs  
Poison Inhalation Hazard: No

#### **IMDG**

UN number: 2224 Class: 6.1  
A, S-A  
Proper shipping name: BENZONITRILE

#### **IATA**

UN number: 2224 Class: 6.1  
Proper shipping name: Benzonitrile

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## **SECTION 15: Regulatory information**

#### **SARA 302 Components**

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

#### **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 1993-02-16
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#### **Pennsylvania Right To Know Components**

benzonitrile	CAS-No. 100-47-0	Revision Date 1993-02-16
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## SECTION 16: Other information

### Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. 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](http://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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