

## SAFETY DATA SHEET

Version 6.9  
Revision Date 08/06/2024  
Print Date 08/07/2024

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Benzonitrile

Product Number : B8959

Brand : SIGALD

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

**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

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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

Combustible liquid.

H302 + H312

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 :  $C_7H_5N$

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**

No data available

### **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**

No data available

### **5.2 Special hazards arising from the substance or mixture**

Carbon oxides

Nitrogen oxides (NO<sub>x</sub>)

Combustible.

### **5.3 Advice for firefighters**

No data available

### **5.4 Further information**

No data available

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## **SECTION 6: Accidental release measures**

### **6.1 Personal precautions, protective equipment and emergency procedures**

For personal protection see section 8.

### **6.2 Environmental precautions**

No data available

### **6.3 Methods and materials for containment and cleaning up**

No data available

### **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**

For precautions see section 2.2.

### **7.2 Conditions for safe storage, including any incompatibilities**

hygroscopic Handle and store under inert gas.

#### **Storage class**

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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

#### Personal protective equipment

##### 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)

##### Control of environmental exposure

Prevent product from entering drains.

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## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

- |                   |                                  |
|-------------------|----------------------------------|
| a) Appearance     | Form: liquid<br>Color: colorless |
| b) Odor           | No data available                |
| c) Odor Threshold | No data available                |

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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 density	3.56 - (Air = 1.0)

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No data available

### 10.2 Chemical stability

No data available

### 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

### 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)
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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)

## 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

No data available

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## SECTION 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

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Proper shipping name: Benzonitrile

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**SECTION 15: Regulatory information****CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
benzonitrile	100-47-0	5000	5000

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

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

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

**SARA 313** : 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.

**US State Regulations****Massachusetts Right To Know**

benzonitrile 100-47-0

**Pennsylvania Right To Know**

benzonitrile 100-47-0

**Maine Chemicals of High Concern**

Product does not contain any listed chemicals

**Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

**Washington Chemicals of High Concern**

Product does not contain any listed chemicals

**The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

**TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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**SECTION 16: Other information**

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

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