

# • SAFETY DATA SHEET

Version 6.8  
Revision Date 01/13/2026  
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## SECTION 1. IDENTIFICATION

### 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 number

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

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

#### Hazards for the product as supplied

Flammable liquids : Category 4

Acute toxicity (Oral) : Category 4

Acute toxicity (Dermal) : Category 4

### Other hazards

None known.

### GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H227 Combustible liquid.  
H302 + H312 Harmful if swallowed or in contact with skin.

Precautionary statements :

**Prevention:**  
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.

**Response:**  
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.

**Storage:**  
P403 + P235 Store in a well-ventilated place. Keep cool.

**Disposal:**  
P501 Dispose of contents/ container to an approved waste disposal plant.

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## SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 100-47-0

## Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
benzotrile	100-47-0*	>= 90 - <= 100	-

\* Indicates that the identifier is a CAS No.

Actual concentration is withheld as a trade secret

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## SECTION 4. FIRST AID MEASURES

- General advice : Show this 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.
- 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
- Protection of first-aiders : For personal protection see section 8.
- Notes to physician : No data available

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## SECTION 5. FIREFIGHTING MEASURES

- 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.
- Specific hazards during fire fighting : Combustible.

Vapours 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.

Hazardous combustion products	: Carbon oxides  Nitrogen oxides (NOx)
Specific extinguishing methods	: No data available
Further information	: Remove container from danger zone and cool with water. Suppress (knock down) gases/vapours/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Do not breathe vapours, 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. Advice for emergency responders: For personal protection see section 8.
Environmental precautions	: Do not let product enter drains.
Methods and materials	: Cover drains. Collect, bind, and pump off spills.

for containment and cleaning up                      Observe possible material restrictions (see sections 7 and 10).  
Take up with liquid-absorbent material (e.g. Chemisorb® ). Dispose of properly. Clean up affected area.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

Advice on protection against fire and explosion                      : Keep away from open flames, hot surfaces and sources of ignition.  
Take precautionary measures against static discharge.

Further information on storage conditions                      : Tightly closed.  
Keep in a well-ventilated place.  
Keep locked up or in an area accessible only to qualified or authorised persons.

Storage class                      : 6.1A, Combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

Recommended storage temperature                      : Recommended storage temperature see product label.

Further information on storage stability                      : hygroscopic  
Handle and store under inert gas.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

**Engineering measures**                      : No data available

### Personal protective equipment

Respiratory protection                      : 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.

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.

#### Hand protection

Material : Viton®  
Break through time : 480 min  
Glove thickness : 0.7 mm  
Protective index : Full contact  
Manufacturer : Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Material : Nitrile rubber  
Break through time : 30 min  
Glove thickness : 0.4 mm  
Protective index : Splash contact  
Manufacturer : Camatril® (KCL 730 / Aldrich Z677442, Size M)

Remarks : 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)).

Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Safety glasses

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance : liquid (68 °F / 20 °C, 1,013 hPa)

Color : colourless

Odor : No data available

Odor Threshold : No data available

pH : No data available

Melting point/ range : 9 °F / -13 °C

	Method: lit.
Boiling point/boiling range	: 376 °F / 191 °C Method: lit.
Flash point	: 158 °F / 70 °C Method: closed cup
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: ca. 1139 °F / 615 °C ca. 1,013 hPa
Upper explosion limit / Upper flammability limit	: 7.2 %(V)
Lower explosion limit / Lower flammability limit	: 1.4 %(V)
Vapor pressure	: 1 hPa (68 °F / 20 °C) 133 hPa (254.3 °F / 123.5 °C)
Relative vapour density	: 3.56 (Air = 1.0)
Relative density	: 1.005
Density	: 1.000 g/cm <sup>3</sup>
Solubility(ies) Water solubility	: 0.001 g/l slightly soluble (77 °F / 25 °C)
Partition coefficient: n- octanol/water	: log Pow: 1.5 (68 °F / 20 °C) Method: OECD Test Guideline 107 GLP: yes Bioaccumulation is not expected.
Autoignition temperature	: 1022 °F / 550 °C
Decomposition temperature	: No data available

#### Viscosity

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Viscosity, dynamic	: 1.24 mPa.s (77 °F / 25 °C)
Viscosity, kinematic	: 1.054 mm <sup>2</sup> /s (100.00 °F / 37.78 °C)
Flow time	: No data available
Explosive properties	: No data available
Oxidizing properties	: none
Surface tension	: 0.03 mN/m, 77 °F / 25 °C
Molecular weight	: 103.12 g/mol
Particle characteristics	
Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

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.
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Violent reactions possible with: Strong oxidizing agents acids
Conditions to avoid	: Avoid moisture. Do not heat over: 30°C  Strong heating.
Incompatible materials	: No data available
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

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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 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.  
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 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

### Ecotoxicity

#### **Components:**

#### **benzonitrile:**

- Toxicity to fish : LC50 (Oncorhynchus mykiss (rainbow trout)): 32 mg/l  
Exposure time: 96 h  
Remarks: (External MSDS)
- Toxicity to algae/aquatic plants : IC50 (Chlorella vulgaris (Fresh water algae)): 231 mg/l  
Exposure time: 6 h  
Test Type: Cell multiplication inhibition test  
Remarks: (IUCLID)
- Toxicity to microorganisms : EC10 (Pseudomonas putida): 11 mg/l  
Exposure time: 16 h  
Remarks: (IUCLID)

#### **Ecotoxicology Assessment**

- Acute aquatic toxicity : This product has no known ecotoxicological effects.
- Chronic aquatic toxicity : This product has no known ecotoxicological effects.

## Persistence and degradability

### Components:

#### benzotrile:

Biodegradability : aerobic  
Inoculum: activated sludge  
Concentration: 12.2 mg/l  
Result: Readily biodegradable.  
Biodegradation: 100 %  
Exposure time: 14 d  
Method: OECD Test Guideline 301E  
GLP: yes

## Bioaccumulative potential

### Components:

#### benzotrile:

Partition coefficient: n- : log Pow: 1.5 (68 °F / 20 °C)  
octanol/water pH: 7.4  
Method: OECD Test Guideline 107  
GLP: yes  
Remarks: Bioaccumulation is not expected.

## Mobility in soil

No data available

## Other adverse effects

No data available

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : 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

### International Regulations

#### IATA-DGR

UN/ID No. : UN 2224  
Proper shipping name : Benzotrile  
Class : 6.1  
Packing group : II  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo : 662  
aircraft)

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Packing instruction : 654  
(passenger aircraft)

**IMDG-Code**

UN number : UN 2224  
Proper shipping name : BENZONITRILE

Class : 6.1  
Packing group : II  
Labels : 6.1  
EmS Code : F-A, S-A  
Marine pollutant : no

**Transport in bulk according to IMO instruments**

Not applicable for product as supplied.

**National Regulations**

**49 CFR Road**

UN/ID/NA number : UN 2224  
Proper shipping name : Benzonitrile

Class : 6.1  
Packing group : II  
Labels : Division 6.1 - Toxic substances  
ERG Code : 152  
Marine pollutant : no

Poison Inhalation Hazard : No

**Special precautions for user**

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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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**

benzotrile 100-47-0

#### **Pennsylvania Right To Know**

benzotrile 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 components 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**

### **Full text of other abbreviations**

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory;

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LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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