

## SAFETY DATA SHEET

Version 5.7  
Revision Date 11/06/2017  
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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Benzonitrile-d<sub>5</sub>

Product Number : 491896  
Brand : Aldrich

CAS-No. : 2102-15-0

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

Identified uses : Laboratory chemicals, Synthesis 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 # : +1-703-527-3887 (CHEMTREC)

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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/doctor if you feel unwell.<br>Rinse mouth.          |
| P302 + P352 + P312 | IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/doctor 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 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 - none

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |                                   |
|------------------|-----------------------------------|
| Synonyms         | : Phenyl-d5 cyanide               |
| Formula          | : C <sub>7</sub> D <sub>5</sub> N |
| Molecular weight | : 108.10 g/mol                    |
| CAS-No.          | : 2102-15-0                       |

#### Hazardous components

| Component              | Classification                                                                                     | Concentration |
|------------------------|----------------------------------------------------------------------------------------------------|---------------|
| <b>Benzonitrile-d5</b> |                                                                                                    |               |
|                        | Flam. Liq. 4; Acute Tox. 4;<br>Skin Irrit. 2; Aquatic Acute 3;<br>H227, H302 + H312, H315,<br>H402 | 90 - 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

No data available

### 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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Store under inert gas. hygroscopic

Storage class (TRGS 510): 6.1B: 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.

Hazardous components without workplace control parameters

### 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.

### 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                                                         |
| 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 | No data available                                                    |
| k) Vapour pressure                              | 1 hPa (1 mmHg) at 20 °C (68 °F)                                      |
| l) Vapour density                               | 3.56 - (Air = 1.0)                                                   |
| m) Relative density                             | 1.059 g/mL at 25 °C (77 °F) 1.059 g/cm <sup>3</sup> at 25 °C (77 °F) |
| 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

Bases, Strong oxidizing agents, Strong reducing agents, Acids, Chlorates, Nitrates, Plastics

### 10.6 Hazardous decomposition products

Other decomposition products - No data available

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO<sub>x</sub>)

In the event of fire: see section 5

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

LC50 Inhalation - Rat - 4 h - 38.6 mg/l

Dermal: No data available

No data available

#### Skin corrosion/irritation

No data available

#### 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.

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: Not available

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

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**12. ECOLOGICAL INFORMATION****12.1 Toxicity**

No data available

**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**

Harmful to aquatic life.

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

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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. Contact a licensed professional waste disposal service to dispose of this material.

**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

**Massachusetts Right To Know Components**

|                 | CAS-No.   | Revision Date |
|-----------------|-----------|---------------|
| Benzonitrile-d5 | 2102-15-0 | 1993-04-24    |

**Pennsylvania Right To Know Components**

|                 | CAS-No.   | Revision Date |
|-----------------|-----------|---------------|
| Benzonitrile-d5 | 2102-15-0 | 1993-04-24    |

|                 | CAS-No.   | Revision Date |
|-----------------|-----------|---------------|
| Benzonitrile-d5 | 2102-15-0 | 1993-04-24    |

**New Jersey Right To Know Components**

|                 | CAS-No.   | Revision Date |
|-----------------|-----------|---------------|
| Benzonitrile-d5 | 2102-15-0 | 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:         | 2 |
| Chronic Health Hazard: |   |
| Flammability:          | 2 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| 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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