

## SAFETY DATA SHEET

Version 4.6  
Revision Date 03/03/2015  
Print Date 11/09/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 1,2-Dicyanobenzene

Product Number : 171719

Brand : Aldrich

CAS-No. : 91-15-6

## 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 # : +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)**

Acute toxicity, Oral (Category 2), H300

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 : Danger

Hazard statement(s)

H300 : Fatal if swallowed.

Precautionary statement(s)

P264 : Wash skin thoroughly after handling.

P270 : Do not eat, drink or smoke when using this product.

P301 + P310 + P330 : IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician. Rinse mouth.

P405 : Store locked up.

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

## 2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

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3. COMPOSITION/INFORMATION ON INGREDIENTS

## 3.1 Substances

Synonyms : Phthalonitrile

Aldrich - 171719

Formula : C<sub>8</sub>H<sub>4</sub>N<sub>2</sub>  
Molecular weight : 128.13 g/mol  
CAS-No. : 91-15-6  
EC-No. : 202-044-8

#### Hazardous components

| Component             | Classification     | Concentration |
|-----------------------|--------------------|---------------|
| <b>Phthalonitrile</b> |                    |               |
|                       | Acute Tox. 2; H300 | <= 100 %      |

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

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## 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. Take victim immediately to hospital. Consult a physician.

#### In case of eye contact

Flush eyes with water as a precaution.

#### If swallowed

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

No data available

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## 6. ACCIDENTAL RELEASE MEASURES

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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust. 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.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. 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 formation of dust and aerosols. Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed.

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.

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

| Component      | CAS-No. | Value                                                    | Control parameters         | Basis                                   |
|----------------|---------|----------------------------------------------------------|----------------------------|-----------------------------------------|
| Phthalonitrile | 91-15-6 | TWA                                                      | 1.000000 mg/m <sup>3</sup> | USA. ACGIH Threshold Limit Values (TLV) |
|                | Remarks | Central Nervous System convulsion<br>body weight effects |                            |                                         |

### 8.2 Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### 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: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

##### Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, 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 particle respirator type N100 (US) or type P3 (EN 143) 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.

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**9. PHYSICAL AND CHEMICAL PROPERTIES****9.1 Information on basic physical and chemical properties**

|                                                 |                                                         |
|-------------------------------------------------|---------------------------------------------------------|
| a) Appearance                                   | Form: crystalline<br>Colour: beige                      |
| b) Odour                                        | No data available                                       |
| c) Odour Threshold                              | No data available                                       |
| d) pH                                           | No data available                                       |
| e) Melting point/freezing point                 | Melting point/range: 137 - 139 °C (279 - 282 °F) - lit. |
| f) Initial boiling point and boiling range      | No data available                                       |
| g) Flash point                                  | 162 °C (324 °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                              | No data available                                       |
| l) Vapour density                               | No data available                                       |
| m) Relative density                             | No data available                                       |
| n) Water solubility                             | No data available                                       |
| o) Partition coefficient: n-octanol/water       | No data available                                       |
| 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**

No data available

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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

No data available

## 10.5 Incompatible materials

Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

## 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 - Rat - 30 mg/kg

Remarks: Behavioral:Tremor. Behavioral:Convulsions or effect on seizure threshold.

Inhalation: No data available

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

Carcinogenicity - Mouse - Oral

Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Liver:Tumors. Leukaemia

Carcinogenicity - Mouse - Skin

Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Leukaemia Tumorigenic Effects: Ovarian tumors.

Carcinogenicity - Mouse - Subcutaneous

Tumorigenic:Equivocal tumorigenic agent by RTECS criteria. Leukaemia Tumorigenic:Tumors at site or application.

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: TI8575000

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

No data available

**12.2 Persistence and degradability**

No data available

**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**

No data available

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**13. DISPOSAL CONSIDERATIONS****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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**14. TRANSPORT INFORMATION****DOT (US)**

UN number: 3439      Class: 6.1      Packing group: II

Proper shipping name: Nitriles, solid, toxic, n.o.s. (Phthalonitrile)

Reportable Quantity (RQ):

Poison Inhalation Hazard: No

**IMDG**

UN number: 3439      Class: 6.1      Packing group: II      EMS-No: F-A, S-A

Proper shipping name: NITRILES, SOLID, TOXIC, N.O.S. (Phthalonitrile)

**IATA**

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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**

Acute Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

Phthalonitrile

CAS-No.  
91-15-6

Revision Date

**New Jersey Right To Know Components**

Phthalonitrile

CAS-No.  
91-15-6

Revision Date

**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      |
| H300       | Fatal if swallowed. |

**HMIS Rating**

|                        |   |
|------------------------|---|
| Health hazard:         | 4 |
| Chronic Health Hazard: |   |
| Flammability:          | 1 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| Fire Hazard:       | 1 |
| 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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