

## SAFETY DATA SHEET

Version 6.2  
Revision Date 09/24/2020  
Print Date 11/19/2020**SECTION 1: Identification of the substance/mixture and of the company/undertaking****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, Synthesis of substances

**1.3 Details of the supplier of the safety data sheet**Company : Sigma-Aldrich Inc.  
3050 Spruce Street  
ST. LOUIS MO 63103  
UNITED STATESTelephone : +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)**

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/ doctor.  
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

---

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms : Phthalonitrile  
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

Component	Classification	Concentration
<b>phthalonitrile</b>		
	Acute Tox. 3; Aquatic Acute 3; Aquatic Chronic 3; H301, H402, H412	<= 100 %

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

---

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Consult a physician. Show this material 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

---

### **SECTION 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

---

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

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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapors, 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.

---

### **SECTION 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): 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

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
phthalonitrile	91-15-6	TWA	1 mg/m <sup>3</sup>	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Central Nervous System convulsion 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: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatril® (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 EC 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.

---

## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |   |   |
|---|---|
| a) Appearance                                   | Form: crystalline<br>Color: beige                       |
| b) Odor   | No data available                                       |
| c) Odor 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) Vapor pressure                               | No data available                                       |
| l) Vapor 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) Autoignition 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

---

## SECTION 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

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

Other decomposition products - No data available

In the event of fire: see section 5

---

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - male and female - 125 mg/kg  
(OECD Test Guideline 401)

#### Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 20 h

Remarks: (ECHA)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation

(OECD Test Guideline 405)

#### Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(OECD Test Guideline 429)

#### Germ cell mutagenicity

Ames test

Salmonella typhimurium

Result: negative

OECD Test Guideline 474

Mouse - male and female

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.

- ACGIH: No ingredient 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 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**

**Specific target organ toxicity - single exposure**

**Specific target organ toxicity - repeated exposure**

**Aspiration hazard**

**Additional Information**

RTECS: Not available

Systemic effects:

After absorption:

Convulsions, Unconsciousness

Symptoms may be delayed.

Other information

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.

Further data:

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

**SECTION 12: Ecological information**

**12.1 Toxicity**

Toxicity to fish	semi-static test LC50 - <i>Oryzias latipes</i> (Orange-red killifish) - 22.6 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - <i>Daphnia magna</i> (Water flea) - 219 mg/l - 48 h (US-EPA)
Toxicity to algae	static test ErC50 - <i>Pseudokirchneriella subcapitata</i> (green algae) - 140 mg/l - 72 h (OECD Test Guideline 201)

**12.2 Persistence and degradability**

Biodegradability	aerobic Dissolved organic carbon (DOC) - Exposure time 28 d Result: 55 % - Not readily biodegradable. (OECD Test Guideline 301E)
Biochemical Oxygen Demand (BOD)	< 10 mg/g Remarks: (External MSDS)
Chemical Oxygen Demand (COD)	1,015 mg/g Remarks: (External MSDS)

### 12.3 Bioaccumulative potential

Bioaccumulation      Cyprinus carpio (Carp) - 42 d  
- 0.2 mg/l(phthalonitrile)

Bioconcentration factor (BCF): < 5.5  
(OECD Test Guideline 305C)

### 12.4 Mobility in soil

### 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

Additional ecological      Biological effects:  
information

When discharged properly, no impairments in the function of adapted biological wastewater treatment plants are to be expected. Further information on ecology  
Discharge into the environment must be avoided.

---

## SECTION 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.

---

## SECTION 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

UN number: 3439      Class: 6.1      Packing group: II  
Proper shipping name: Nitriles, solid, toxic, n.o.s. (phthalonitrile)

---

## SECTION 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 the State of California to cause cancer, birth, or any other reproductive defects.

---

## **SECTION 16: Other information**

### **Further information**

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. 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.

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).

Version: 6.2

Revision Date: 09/24/2020

Print Date: 11/19/2020