

## SAFETY DATA SHEET

Version 5.1

Revision Date 07/01/2014

Print Date 11/14/2018

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1. PRODUCT AND COMPANY IDENTIFICATION

## 1.1 Product identifiers

Product name : 2-Phenylbutyronitrile

Product Number : 222739

Brand : Aldrich

CAS-No. : 769-68-6

## 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 4), H302

Acute toxicity, Inhalation (Category 4), H332

Acute toxicity, Dermal (Category 4), H312

Acute aquatic toxicity (Category 3), H402

Chronic aquatic toxicity (Category 3), H412

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)

H302 + H312 + H332

H412

Harmful if swallowed, in contact with skin or if inhaled

Harmful to aquatic life with long lasting effects.

Precautionary statement(s)

P261

P264

P270

P271

P273

P280

P301 + P312

Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.

Wash skin thoroughly after handling.

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

Use only outdoors or in a well-ventilated area.

Avoid release to the environment.

Wear protective gloves/ protective clothing.

IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you

|             |                                                                                                                                                     |
|-------------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| P302 + P352 | feel unwell.                                                                                                                                        |
| P304 + P340 | IF ON SKIN: Wash with plenty of soap and water.<br>IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing. |
| P312        | Call a POISON CENTER or doctor/ physician if you feel unwell.                                                                                       |
| P322        | Specific measures (see supplemental first aid instructions on this label).                                                                          |
| P330        | Rinse mouth.                                                                                                                                        |
| P363        | Wash contaminated clothing before reuse.                                                                                                            |
| 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 :  $\alpha$ -Ethylphenylacetonitrile

Formula :  $C_{10}H_{11}N$   
Molecular Weight : 145.2 g/mol  
CAS-No. : 769-68-6  
EC-No. : 212-213-8

#### Hazardous components

| Component                       | Classification                                                                   | Concentration |
|---------------------------------|----------------------------------------------------------------------------------|---------------|
| <b>DL-2-Phenylbutyronitrile</b> |                                                                                  |               |
|                                 | Acute Tox. 4; Aquatic Acute 3;<br>Aquatic Chronic 3; H302 +<br>H312 + H332, H412 | -             |

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

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

## 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 (NOx), Hydrogen cyanide (hydrocyanic acid)
- 5.3 Advice for firefighters**  
Wear self contained breathing apparatus for fire fighting 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**  
Use personal protective equipment. Avoid breathing vapours, mist or gas. Ensure adequate ventilation.  
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**  
Soak up with inert absorbent material and dispose of as hazardous waste. 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.  
Normal measures for preventive fire protection.  
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.
- 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.
- 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<br>Colour: colourless                     |
| b) Odour                                        | no data available                                      |
| c) Odour Threshold                              | no data available                                      |
| d) pH                                           | no data available                                      |
| e) Melting point/freezing point                 | no data available                                      |
| f) Initial boiling point and boiling range      | 114 - 115 °C (237 - 239 °F) at 20 hPa (15 mmHg) - lit. |
| g) Flash point                                  | 105 °C (221 °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                             | 0.974 g/cm <sup>3</sup> at 25 °C (77 °F)               |
| n) Water solubility                             | no data available                                      |
| o) Partition coefficient: n-octanol/water       | log Pow: 2.547                                         |
| 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 oxidizing 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**

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.

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: 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

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

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

Harmful to aquatic life.

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)

Not dangerous goods

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

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## 15. REGULATORY INFORMATION

### SARA 302 Components

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

### SARA 313 Components

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.

### 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

DL-2-Phenylbutyronitrile

CAS-No.  
769-68-6

Revision Date

### New Jersey Right To Know Components

DL-2-Phenylbutyronitrile

CAS-No.  
769-68-6

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                                           |
| Aquatic Acute      | Acute aquatic toxicity                                   |
| Aquatic Chronic    | Chronic aquatic toxicity                                 |
| H302               | Harmful if swallowed.                                    |
| H302 + H312 + H332 | Harmful if swallowed, in contact with skin or if inhaled |

### HMIS Rating

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

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 1 |
| Fire Hazard:       | 1 |
| Reactivity Hazard: | 0 |

### Further information

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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.

### Preparation Information

Sigma-Aldrich Corporation  
Product Safety – Americas Region  
1-800-521-8956

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