

## SAFETY DATA SHEET

Version 4.5  
Revision Date 10/27/2017  
Print Date 11/09/2018

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**1. PRODUCT AND COMPANY IDENTIFICATION****1.1 Product identifiers**

Product name : Allyl cyanide

Product Number : 122793

Brand : Aldrich

CAS-No. : 109-75-1

**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 3), H226

Acute toxicity, Oral (Category 3), H301

Acute toxicity, Inhalation (Category 3), H331

Acute toxicity, Dermal (Category 4), H312

Skin irritation (Category 2), H315

Eye irritation (Category 2A), H319

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)

H226

Flammable liquid and vapour.

H301 + H331

Toxic if swallowed or if inhaled

H312

Harmful in contact with skin.

H315

Causes skin irritation.

H319

Causes serious eye irritation.

Precautionary statement(s)

P210

Keep away from heat/sparks/open flames/hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

|                    |  |
|--------------------|--|
| P241               | Use explosion-proof electrical/ ventilating/ lighting/ equipment.  |
| P242               | Use only non-sparking tools.   |
| P243               | Take precautionary measures against static discharge.  |
| P261               | Avoid breathing dust/ fume/ gas/ mist/ vapours/ spray.   |
| P264               | Wash skin thoroughly after handling.   |
| P270               | Do not eat, drink or smoke when using this product.  |
| P271               | Use only outdoors or in a well-ventilated area.  |
| P280               | Wear protective gloves/ eye protection/ face protection.   |
| P301 + P310 + P330 | IF SWALLOWED: Immediately call a POISON CENTER/doctor. Rinse mouth.  |
| P303 + P361 + P353 | IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower.                              |
| P304 + P340 + P311 | IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/doctor.                          |
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| P332 + P313        | If skin irritation occurs: Get medical advice/ attention.  |
| P337 + P313        | If eye irritation persists: 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 + P233        | Store in a well-ventilated place. Keep container tightly closed.   |
| P403 + P235        | Store in a well-ventilated place. Keep cool.   |
| 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

## 3. COMPOSITION/INFORMATION ON INGREDIENTS

### 3.1 Substances

|                  |  |
|------------------|--|
| Synonyms         | : 3-Butenenitrile<br>Vinylacetonitrile |
| Formula          | : C <sub>4</sub> H <sub>5</sub> N      |
| Molecular weight | : 67.09 g/mol                          |
| CAS-No.          | : 109-75-1                             |
| EC-No.           | : 203-701-1                            |

#### Hazardous components

| Component               | Classification   | Concentration |
|-------------------------|--|---------------|
| <b>But-3-enenitrile</b> |  |               |
|                         | Flam. Liq. 3; Acute Tox. 3;<br>Acute Tox. 4; Skin Irrit. 2; Eye<br>Irrit. 2A; H226, H301 + H331,<br>H312, H315, H319 | 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. Take victim immediately to hospital. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**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**

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. 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.

**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).

**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.

Storage class (TRGS 510): 3: Flammable liquids

**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

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: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, Size M)

#### Splash contact

Material: butyl-rubber

Minimum layer thickness: 0.3 mm

Break through time: 480 min

Material tested: Butoject® (KCL 897 / Aldrich Z677647, 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, Flame retardant antistatic protective clothing., 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.

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## 9. PHYSICAL AND CHEMICAL PROPERTIES

### 9.1 Information on basic physical and chemical properties

- |  |   |
|--|---|
| a) Appearance                              | Form: clear, liquid<br>Colour: light yellow |
| 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 | 116 - 121 °C (241 - 250 °F) - lit.          |
| g) Flash point                             | 24 °C (75 °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                             | 0.834 g/cm <sup>3</sup> at 25 °C (77 °F) |
| 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

Vapours may form explosive mixture with air.

### 10.4 Conditions to avoid

Heat, flames and sparks.

### 10.5 Incompatible materials

Oxidizing agents, Strong acids, Strong bases, 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

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## 11. TOXICOLOGICAL INFORMATION

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - Rat - 115 mg/kg

LD50 Dermal - Rabbit - 1,176 mg/kg

No data available

#### Skin corrosion/irritation

Skin - Rabbit

Result: Open irritation test - 24 h

#### 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

Reproductive toxicity - Rat - Inhalation

Effects on Fertility: Post-implantation mortality (e.g., dead and/or resorbed implants per total number of implants). Effects on Embryo or Fetus: Fetotoxicity (except death, e.g., stunted fetus).

No data available

Developmental Toxicity - Rat - Inhalation

Specific Developmental Abnormalities: Craniofacial (including nose and tongue). Specific Developmental Abnormalities: Musculoskeletal system.

**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: EM8050000

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**

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 182 mg/l - 96 h

**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

Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. 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: 1992      Class: 3 (6.1)      Packing group: III  
Proper shipping name: Flammable liquids, toxic, n.o.s. (But-3-enenitrile)  
Reportable Quantity (RQ):  
Poison Inhalation Hazard: No

#### IMDG

UN number: 1992      Class: 3 (6.1)      Packing group: III      EMS-No: F-E, S-D  
Proper shipping name: FLAMMABLE LIQUID, TOXIC, N.O.S. (But-3-enenitrile)

#### IATA

UN number: 1992      Class: 3 (6.1)      Packing group: III  
Proper shipping name: Flammable liquid, toxic, n.o.s. (But-3-enenitrile)

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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

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

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

#### Pennsylvania Right To Know Components

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| But-3-enenitrile | 109-75-1 |               |

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| But-3-enenitrile | 109-75-1 |               |

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| But-3-enenitrile | 109-75-1 |               |

#### New Jersey Right To Know Components

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| But-3-enenitrile | 109-75-1 |               |

|                  | CAS-No.  | Revision Date |
|------------------|----------|---------------|
| But-3-enenitrile | 109-75-1 |               |

**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                   |
| Eye Irrit.  | Eye irritation                   |
| Flam. Liq.  | Flammable liquids                |
| H226        | Flammable liquid and vapour.     |
| H301        | Toxic if swallowed.              |
| H301 + H331 | Toxic if swallowed or if inhaled |
| H312        | Harmful in contact with skin.    |
| H315        | Causes skin irritation.          |
| H319        | Causes serious eye irritation.   |

**HMIS Rating**

|                        |   |
|------------------------|---|
| Health hazard:         | 4 |
| Chronic Health Hazard: |   |
| Flammability:          | 3 |
| Physical Hazard        | 0 |

**NFPA Rating**

|                    |   |
|--------------------|---|
| Health hazard:     | 4 |
| Fire Hazard:       | 3 |
| 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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