

### 1. PRODUCT AND COMPANY IDENTIFICATION

#### 1.1 Product identifiers

Product name : 4,5-Dimethoxy-2-nitrobenzotrile

Product Number : 650102  
Brand : Aldrich

CAS-No. : 102714-71-6

#### 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)

### 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  
Skin irritation (Category 2), H315  
Eye irritation (Category 2A), H319  
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335

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  
H315  
H319  
H335

Harmful if swallowed, in contact with skin or if inhaled  
Causes skin irritation.  
Causes serious eye irritation.  
May cause respiratory irritation.

Precautionary statement(s)

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 + P312        | IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell.  |
| P302 + P352        | IF ON SKIN: Wash with plenty of soap and water.  |
| P304 + P340        | IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.                                 |
| P305 + P351 + P338 | IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. |
| 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.   |
| 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.  |
| P403 + P233        | Store in a well-ventilated place. Keep container tightly closed.   |
| 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

|                  |   |
|------------------|---|
| Formula          | : C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> |
| Molecular Weight | : 208.17 g/mol  |
| CAS-No.          | : 102714-71-6   |

#### Hazardous components

| Component                              | Classification  | Concentration |
|--|---|---------------|
| <b>4,5-Dimethoxy-2-nitrobenzotrile</b> |   |               |
|  | Acute Tox. 4; Skin Irrit. 2; Eye Irrit. 2A; STOT SE 3; H302 + H312 + H332, H315, H319, H335 | -             |

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

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

#### 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 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 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

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.

Provide appropriate exhaust ventilation at places where dust is formed. 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.

### 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

Safety glasses with side-shields conforming to EN166 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

For nuisance exposures use type P95 (US) or type P1 (EU EN 143) particle respirator. For higher level protection use type OV/AG/P99 (US) or type ABEK-P2 (EU EN 143) respirator cartridges. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### Control of environmental exposure

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: solid   |
| b) Odour  | no data available                                       |
| c) Odour Threshold                              | no data available                                       |
| d) pH   | no data available                                       |
| e) Melting point/freezing point                 | Melting point/range: 164 - 168 °C (327 - 334 °F) - lit. |
| f) Initial boiling point and boiling range      | no data available                                       |
| g) Flash point                                  | no data available                                       |
| 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 oxidizing agents, Strong bases

### 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

Inhalation - May cause respiratory irritation.

#### 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

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.

#### 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

4,5-Dimethoxy-2-nitrobenzotrile

CAS-No.  
102714-71-6

Revision Date

### New Jersey Right To Know Components

4,5-Dimethoxy-2-nitrobenzotrile

CAS-No.  
102714-71-6

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   |
| Eye Irrit.         | Eye irritation   |
| H302               | Harmful if swallowed.                                    |
| H302 + H312 + H332 | Harmful if swallowed, in contact with skin or if inhaled |
| H312               | Harmful in contact with skin.                            |
| H315               | Causes skin irritation.                                  |
| H319               | Causes serious eye irritation.                           |

### HMIS Rating

|                        |   |
|------------------------|---|
| Health hazard:         | 2 |
| Chronic Health Hazard: |   |
| Flammability:          | 0 |
| Physical Hazard        | 0 |

### NFPA Rating

|                    |   |
|--------------------|---|
| Health hazard:     | 2 |
| Fire Hazard:       | 0 |
| 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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