

## SAFETY DATA SHEET

Version 6.0  
Revision Date 09/28/2019  
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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 3-(4-Bromophenyl)isoxazole-5-carboxaldehyde

Product Number : 717843  
Brand : Aldrich  
CAS-No. : 863391-64-4

**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 ST  
ST. LOUIS MO 63103  
UNITED STATES

Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

**1.4 Emergency telephone number**

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 4), H302

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 : Harmful if swallowed.

|                            |                                                                     |
|----------------------------|---------------------------------------------------------------------|
| Precautionary statement(s) |                                                                     |
| P264                       | Wash skin thoroughly after handling.                                |
| P270                       | Do not eat, drink or smoke when using this product.                 |
| P301 + P312                | IF SWALLOWED: Call a POISON CENTER/doctor if you feel unwell.       |
| P330                       | Rinse mouth.                                                        |
| 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

|                  |                                                    |
|------------------|----------------------------------------------------|
| Formula          | : C <sub>10</sub> H <sub>6</sub> BrNO <sub>2</sub> |
| Molecular weight | : 252.06 g/mol                                     |
| CAS-No.          | : 863391-64-4                                      |

| Component                                          | Classification     | Concentration |
|----------------------------------------------------|--------------------|---------------|
| <b>3-(4-Bromophenyl)isoxazole-5-carboxaldehyde</b> |                    |               |
|                                                    | Acute Tox. 4; H302 | <= 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 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

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## **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>), Hydrogen bromide gas

### **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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## **SECTION 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. 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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## **SECTION 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.  
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.

Recommended storage temperature 2 - 8 °C

Storage class (TRGS 510): 13: Non Combustible Solids

### **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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## **SECTION 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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## SECTION 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: 162 - 166 °C (324 - 331 °F) |
| 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                            | 8.7 - (Air = 1.0) |
| m) | Relative density                          | No data available |
| n) | Water solubility                          | No data available |
| o) | Partition coefficient:<br>n-octanol/water | log Pow: 2.994    |
| p) | Auto-ignition<br>temperature              | No data available |
| q) | Decomposition<br>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

|                            |                   |
|----------------------------|-------------------|
| Relative vapour<br>density | 8.7 - (Air = 1.0) |
|----------------------------|-------------------|

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## 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 oxidizing agents

### 10.6 Hazardous decomposition products

Other decomposition products - No data available

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

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

No data available

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**

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 on OSHA's list of regulated carcinogens.

**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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**SECTION 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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## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

#### Product

Offer surplus and non-recyclable solutions to a licensed disposal company.

#### Contaminated packaging

Dispose of as unused product.

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## SECTION 14: Transport information

### DOT (US)

Not dangerous goods

### IMDG

Not dangerous goods

### IATA

Not dangerous goods

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## 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

3-(4-Bromophenyl)isoxazole-5-carboxaldehyde

CAS-No.  
863391-64-4

Revision Date

### New Jersey Right To Know Components

3-(4-Bromophenyl)isoxazole-5-carboxaldehyde

CAS-No.  
863391-64-4

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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**SECTION 16: Other information****Further information**

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