

## Chemical Safety Data Sheet MSDS / SDS

**3-Bromo-4-isopropoxy-5-methoxybenzotrile**Revision Date:2026-05-31 Revision Number:1

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 3-Bromo-4-isopropoxy-5-methoxybenzotrile  
CBnumber : CB31116484  
CAS : 515848-62-1  
Synonyms : Albb-008952;3-bromo-5-methoxy-4-propan-2-yloxybenzotrile

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

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**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P405 Store locked up.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

**Hazard statements**

H335 May cause respiratory irritation

H331 Toxic if inhaled

H319 Causes serious eye irritation

H315 Causes skin irritation

H312 Harmful in contact with skin

H302 Harmful if swallowed

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 3-Bromo-4-isopropoxy-5-methoxybenzotrile
Synonyms	: Albb-008952;3-bromo-5-methoxy-4-propan-2-yloxybenzotrile
CAS	: 515848-62-1
MF	: C11H12BrNO2
MW	: 270.12

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## SECTION 4: First aid measures

### General Advice

If symptoms persist, call a physician.

### Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

### Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

### Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

### Ingestion

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

### Most important symptoms and effects

None reasonably foreseeable.

### Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

### Notes to Physician

Treat symptomatically.

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## SECTION 5: Firefighting measures

### Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

### Extinguishing media which must not be used for safety reasons

No information available.

### Specific Hazards Arising from the Chemical

Thermal decomposition can lead to release of irritating gases and vapors.

### Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

### NFPA 704



**HEALTH 2** Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

**FIRE 1** Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

**SPEC.**

**HAZ.**

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## SECTION 6: Accidental release measures

### Personal Precautions

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

### Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

### Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

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## SECTION 7: Handling and storage

## Handling

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

## Storage

Keep container tightly closed in a dry and well-ventilated place.

## Specific Use(s)

Use in laboratories

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## SECTION 8: Exposure controls/personal protection

### Control Parameters

### Monitoring methods

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust

### Exposure Controls

### Engineering Measures

Ensure that eyewash stations and safety showers are close to the workstation location. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

### Personal protective equipment

#### Eye Protection

Goggles (European standard - EN 166)

#### Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.

(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g.

sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

### **Skin and body protection**

Long sleeved clothing

### **Respiratory Protection**

When workers are facing concentrations above the exposure limit they must use appropriate certified respirators.

To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

### **Large scale/emergency use**

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Recommended Filter type: Particulates filter conforming to EN 143

### **Small scale/Laboratory use**

Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended half mask:- Particle filtering: EN149:2001

When RPE is used a face piece Fit Test should be conducted

### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

### **Environmental exposure controls**

No information available.

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## SECTION 9: Physical and chemical properties

### **Information on basic physicochemical properties**

No information available

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### **Physical State**

Solid

### **Odor**

No information av

### **Odor Threshold**

No data available

### **pH**

No information av

### **Melting Point/Range**

No data available

### **Softening Point**

No data available

### **Boiling Point/Range**

No information available

### **Flash Point**

No information available

Method - No information available

### **Evaporation Rate**

Not applicable Solid

### **Flammability (solid,gas)**

No information available

### **Explosion Limits**

No data available

### **Vapor Pressure**

No data available

### **Vapor Density**

Not applicable Solid

### **Specific Gravity / Density**

No data available

### **Bulk Density**

No data available

### **Water Solubility**

No information available

### **Solubility in other solvents**

No information available

### **Partition Coefficient (n-octanol/water)**

No data available

### **Autoignition Temperature**

No data available

### **Decomposition Temperature**

No data available

### **Viscosity**

Not applicable Solid

### **Explosive Properties**

No information available

### **Oxidizing Properties**

No information available

### **Molecular Formula**

C11 H12 Br N O2

### **Molecular Weight**

270.13

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## SECTION 10: Stability and reactivity

### **Stability**

Stable under normal conditions.

### **Hazardous Reactions**

None under normal processing.

### **Hazardous Polymerization**

No information available.

### **Conditions to Avoid**

None known.

### **Materials to avoid**

No information available.

### **Hazardous Decomposition Products**

None under normal use conditions.

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## SECTION 11: Toxicological information

### **Product Information**

**(a) acute toxicity;**

**(b) skin corrosion/irritation;**

Category 2

**(c) serious eye damage/irritation;**

Category 2

**(d) respiratory or skin sensitization;**

**Respiratory**

No data available

**Skin**

No data available

**(e) germ cell mutagenicity;**

No data available

**(f) carcinogenicity;**

No data available

There are no known carcinogenic chemicals in this product

**(g) reproductive toxicity;**

No data available

**(h) STOT-single exposure;**

Category 3

**Results / Target organs**

Respiratory system

**(i) STOT-repeated exposure;**

No data available

**Target Organs**

No information available.

**(j) aspiration hazard;**

Not applicable

Solid

**Symptoms / effects, both acute and delayed**

No information available

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## SECTION 12: Ecological information

**Ecotoxicity effects**

Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

**Persistence and Degradability**

No information available

**Bioaccumulative Potential**

No information available

**Mobility in soil**

No information available

## Endocrine Disruptor Information

This product does not contain any known or suspected endocrine disruptors

## Persistent Organic Pollutant

This product does not contain any known or suspected substance

## Ozone Depletion Potential

This product does not contain any known or suspected substance

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# SECTION 13: Disposal considerations

## Waste from Residues/Unused Products

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

## Contaminated Packaging

Dispose of this container to hazardous or special waste collection point.

## Other Information

Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

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# SECTION 14: Transport information

## Road and Rail Transport

### UN-No

UN3439

### Proper Shipping Name

NITRILES, SOLID, TOXIC, N.O.S.

### Technical Shipping Name

(3-Bromo-4-isopropoxy-5-methoxybenzotrile)

### Hazard Class

6.1

### Packing Group

III

## IMDG/IMO

### UN-No

UN3439

### Proper Shipping Name

NITRILES, SOLID, TOXIC, N.O.S.

### Technical Shipping Name

(3-Bromo-4-isopropoxy-5-methoxybenzotrile)

**Hazard Class**

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**IATA****UN-No**

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**Proper Shipping Name**

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**Technical Shipping Name**

(3-Bromo-4-isopropoxy-5-methoxybenzotrile)

**Hazard Class**

6.1

**Packing Group**

III

**Special Precautions for User**

No special precautions required

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## SECTION 15: Regulatory information

**International Inventories**

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

**National Regulations**

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## SECTION 16: Other information

**Prepared By**

Health, Safety and Environmental Department

**Revision Date**

16-Oct-2025

**Revision Summary**

Not applicable.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene. Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

## **Legend**

### **CAS**

Chemical Abstracts Service

### **TSCA**

United States Toxic Substances Control Act Section 8(b)

Inventory

### **EINECS/ELINCS**

European Inventory of Existing Commercial Chemical

Substances/EU List of Notified Chemical Substances

### **DSL/NDSL**

Canadian Domestic Substances List/Non-Domestic

Substances List

### **PICCS**

Philippines Inventory of Chemicals and Chemical Substances

### **ENCS**

Japanese Existing and New Chemical Substances

### **IECSC**

Chinese Inventory of Existing Chemical Substances

### **AICS**

Australian Inventory of Chemical Substances

### **KECL**

Korean Existing and Evaluated Chemical Substances

### **NZIoC**

New Zealand Inventory of Chemicals

### **WEL**

Workplace Exposure Limit

### **TWA**

Time Weighted Average

### **ACGIH**

American Conference of Governmental Industrial Hygienists

### **IARC**

International Agency for Research on Cancer

### **DNEL**

Derived No Effect Level

### **PNEC**

Predicted No Effect Concentration

### **RPE**

Respiratory Protective Equipment

### **LD50**

Lethal Dose 50%

### **LC50**

Lethal Concentration 50%

**EC50**

Effective Concentration 50%

**NOEC**

No Observed Effect Concentration

**POW**

Partition coefficient Octanol:Water

**PBT**

Persistent, Bioaccumulative, Toxic

**vPvB**

very Persistent, very Bioaccumulative

**ICAO/IATA**

International Civil Aviation Organization/International Air  
Transport Association

**IMO/IMDG**

International Maritime Organization/International Maritime  
Dangerous Goods Code

**ADR**

European Agreement Concerning the International Carriage of  
Dangerous Goods by Road

**MARPOL**

International Convention for the Prevention of Pollution from  
Ships

**OECD**

Organisation for Economic Co-operation and Development

**ATE**

Acute Toxicity Estimate

**BCF**

Bioconcentration factor

**VOC**

(Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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