

## Chemical Safety Data Sheet MSDS / SDS

**4-BROMO-2,2-DIPHENYLBUTYRONITRILE**

Revision Date:2026-05-31 Revision Number:1

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

Product name : 4-BROMO-2,2-DIPHENYLBUTYRONITRILE  
CBnumber : CB0434881  
CAS : 39186-58-8  
EINECS Number : 254-337-5  
Synonyms : 4-bromo-2,2-diphenylbutanenitrile, 4-BROMO-2,2-DIPHENYLBUTYRONITRILE

**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

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

Symbol(GHS)



Signal word

Warning

**Precautionary statements**

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

P405 Store locked up.

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/protective clothing/eye protection/face protection.

P501 Dispose of contents/container to.....

**Hazard statements**

H315 Causes skin irritation

H319 Causes serious eye irritation

H302 Harmful if swallowed

H312 Harmful in contact with skin

H331 Toxic if inhaled

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## SECTION 3: Composition/information on ingredients

### Substance

|              |                                                                        |
|--------------|------------------------------------------------------------------------|
| Product name | : 4-BROMO-2,2-DIPHENYLBUTYRONITRILE                                    |
| Synonyms     | : 4-bromo-2,2-diphenylbutanenitrile, 4-BROMO-2,2-DIPHENYLBUTYRONITRILE |
| CAS          | : 39186-58-8                                                           |
| EC number    | : 254-337-5                                                            |
| MF           | : C <sub>16</sub> H <sub>14</sub> BrN                                  |
| MW           | : 300.2                                                                |

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## SECTION 4: First aid measures

### Eye Contact

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

### Skin Contact

Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes.

### Inhalation

Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration.

### Ingestion

Clean mouth with water. Get medical attention.

### Most important symptoms and effects

No information available.

### 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.

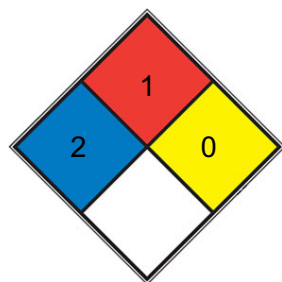
### Specific Hazards Arising from the Chemical

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.

## SECTION 6: Accidental release measures

### Personal Precautions

Ensure adequate ventilation.

### Environmental Precautions

See Section 12 for additional Ecological Information.

### Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: Handling and storage

## Handling

Avoid contact with skin and eyes. Avoid contact with skin and clothing. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Avoid breathing vapors or mists. Do not ingest. If swallowed then seek immediate medical assistance. Wash thoroughly after handling.

## Storage

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

## 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 adequate ventilation, especially in confined areas. Ventilation systems. 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

Wear safety glasses with side shields (or 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**

No protective equipment is needed under normal use conditions.

#### **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

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

Maintain adequate ventilation

#### **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**

Off-white

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#### **Physical State**

Powder Solid

#### **Odor**

Odorless

#### **Odor Threshold**

No data available

#### **pH**

6.3 saturated sol

#### **Melting Point/Range**

64 - 69 °C / 147.2 - 156.2 °F

#### **Softening Point**

No data available

#### **Boiling Point/Range**

160 - 165 °C / 320 - 329 °F @ 0.2 MBAR

#### **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**

0Pa at 20°C

### **Vapor Density**

Not applicable Solid

### **Specific Gravity / Density**

1.4184 (rough estimate)

### **Bulk Density**

1.4184 (rough estimate)

### **Water Solubility**

10 mg/l

### **Solubility in other solvents**

Chloroform (Slightly) Ethyl Acetate (Slightly)

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

No data available

### **desc\_info**

Component: 4-Bromo-2,2-diphenylbutanenitrile log Pow: 4.2

### **Autoignition Temperature**

520 °C / 968 °F

### **Decomposition Temperature**

No data available

### **Viscosity**

Not applicable Solid

### **Explosive Properties**

No information available

### **Oxidizing Properties**

No information available

### **Molecular Formula**

C16 H14 Br N

### **Molecular Weight**

300.19

### **Colour**

White

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## SECTION 10: Stability and reactivity

### **Stability**

Stable under normal conditions.

### **Hazardous Reactions**

No information available.

### **Hazardous Polymerization**

No information available.

### **Conditions to Avoid**

Incompatible products.

### **Materials to avoid**

Strong oxidizing agents. Strong acids. Strong bases.

### **Hazardous Decomposition Products**

Nitrogen oxides (NO<sub>x</sub>). Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Hydrogen halides.

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## SECTION 11: Toxicological information

### **Product Information**

**(a) acute toxicity;**

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

No data available

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

No data available

**(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;**

No data available

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

No data available

**Target Organs**

No information available.

**(j) aspiration hazard;**

Not applicable

Solid

**Other Adverse Effects**

The toxicological properties have not been fully investigated.

**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**

**Persistence**

Soluble in water, Persistence is unlikely, based on information available.

**Bioaccumulative Potential**



Bioaccumulation is unlikely

| Component                         | log Pow | Bioconcentration factor (BCF) |
|-----------------------------------|---------|-------------------------------|
| 4-Bromo-2,2-diphenylbutanenitrile | 4.2     | No data available             |

### Mobility in soil

The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils

### 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

Not Regulated

### IMDG/IMO

Not regulated

### IATA

Not regulated

### Special Precautions for User

No special precautions required

## 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).

| Component             | The Inventory of Hazardous Chemicals (2015 Edition) | List of dangerous goods GB 12268 - 2012 | TCS | IECSC | EINECS    | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL |
|-----------------------|-----------------------------------------------------|-----------------------------------------|-----|-------|-----------|------|-----|-------|------|------|------|------|
| 4-Bromo-2,2-diphenylb | -                                                   | -                                       | X   | -     | 254-337-5 | -    | -   | -     | -    | -    | -    | -    |

|          |             |          |
|----------|-------------|----------|
|          | utan        | enitrile |
| National | Regulations |          |

## SECTION 16: Other information

### Prepared By

Health, Safety and Environmental Department

### Revision Date

15-Sep-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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