

ALFAAA17786

## 4-Bromo-2,2-diphenylbutyronitrile

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

<b>产品说明:</b> <b>Product Description:</b>	<b>4-溴-2,2-二苯丁腈</b> <b>4-Bromo-2,2-diphenylbutyronitrile</b>
<b>Cat No. :</b>	<b>A17786</b>
<b>Synonyms</b>	\$1-(2-Bromoethyl)-\$1-phenylbenzeneacetonitrile
<b>CAS No</b>	39186-58-8
<b>Molecular Formula</b>	C16 H14 Br N
<b>Supplier</b>	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
<b>Emergency Telephone Number</b>	For information <b>US</b> call: 001-800-227-6701 / <b>Europe</b> call: +32 14 57 52 11 Emergency Number <b>US</b> :001-201-796-7100 / <b>Europe</b> : +32 14 57 52 99 <b>CHEMTREC</b> Tel. No. <b>US</b> :001-800-424-9300 / <b>Europe</b> :001-703-527-3887
<b>E-mail address</b>	begel.sdsdesk@thermofisher.com
<b>Recommended Use</b> <b>Uses advised against</b>	Laboratory chemicals. No Information available

### SECTION 2. HAZARD IDENTIFICATION

<b>Physical State</b> Powder Solid	<b>Appearance</b> Off-white	<b>Odor</b> Odorless
<b>Emergency Overview</b> Harmful if swallowed.		

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 4
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#### Label Elements



**Signal Word**

**Warning**

#### **Hazard Statements**

H302 - Harmful if swallowed

**Precautionary Statements****Prevention**

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

**Response**

P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

**Storage**

P403 - Store in a well-ventilated place

**Disposal**

P501 - Dispose of contents/ container to an approved waste disposal plant

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Harmful if swallowed.

**Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
4-Bromo-2,2-diphenylbutanenitrile	39186-58-8	95

**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.

**SECTION 5. FIRE-FIGHTING 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.

**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

**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 Neoprene Natural rubber PVC	See manufacturers recommendations	-	EN 374	(minimum requirement)

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.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

<b>Appearance</b>	Off-white	
<b>Physical State</b>	Powder Solid	
<b>Odor</b>	Odorless	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	6.3	saturated sol
<b>Melting Point/Range</b>	64 - 69 °C / 147.2 - 156.2 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	160 - 165 °C / 320 - 329 °F	@ 0.2 MBAR
<b>Flash Point</b>	No information available	<b>Method -</b> No information available
<b>Evaporation Rate</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Specific Gravity / Density</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Water Solubility</b>	10 mg/l	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Component</b>	<b>log Pow</b>	
4-Bromo-2,2-diphenylbutanenitrile	4.2	
<b>Autoignition Temperature</b>	520 °C / 968 °F	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	Not applicable	Solid
<b>Explosive Properties</b>	No information available	
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C16 H14 Br N	

# SAFETY DATA SHEET

## 4-Bromo-2,2-diphenylbutyronitrile

Molecular Weight 300.19

### 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.

### 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

### SECTION 12. ECOLOGICAL INFORMATION

# SAFETY DATA SHEET

## 4-Bromo-2,2-diphenylbutyronitrile

**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

### 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.

### 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	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
4-Bromo-2,2-diphenylb	-	-	X	-	254-337-5	-	-	-	-		-	-

## 4-Bromo-2,2-diphenylbutyronitrile

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## National Regulations

## SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department  
Revision Date 27-Apr-2024  
Revision Summary New emergency telephone response service provider.

## 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

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**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

## Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

**End of Safety Data Sheet**