

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description: **3-Bromo-4-methoxybenzotrile**
 Cat No. : **429880000; 429880010; 429880100**
 CAS No **117572-79-9**
 Molecular Formula **C8 H6 Br N O**

1.2. Relevant identified uses of the substance or mixture and uses advised against

Recommended Use Laboratory chemicals.
 Uses advised against No Information available

1.3. Details of the supplier of the safety data sheet

Company

UK entity/business name
 Fisher Scientific UK
 Bishop Meadow Road,
 Loughborough, Leicestershire LE11 5RG, United Kingdom

EU entity/business name
 Thermo Fisher Scientific
 Janssen Pharmaceuticaaan 3a, 2440 Geel, Belgium

E-mail address begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Based on available data, the classification criteria are not met

Health hazards

Acute oral toxicity Category 4 (H302)
 Acute dermal toxicity Category 4 (H312)

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Acute Inhalation Toxicity - Dusts and Mists
Skin Corrosion/Irritation
Serious Eye Damage/Eye Irritation
Specific target organ toxicity - (single exposure)

Category 4 (H332)
Category 2 (H315)
Category 2 (H319)
Category 3 (H335)

Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H319 - Causes serious eye irritation
H315 - Causes skin irritation
H335 - May cause respiratory irritation
H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements

P280 - Wear protective gloves/protective clothing/eye protection/face protection
P302 + P352 - IF ON SKIN: Wash with plenty of soap and water
P261 - Avoid breathing dust/fume/gas/mist/vapors/spray
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing
P280 - Wear protective gloves/protective clothing/eye protection/face protection
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
3-Bromo-4-methoxybenzonitrile	117572-79-9		>95	STOT SE 3 (H335) Skin Irrit. 2 (H315) Eye Irrit. 2 (H319) Acute Tox. 4 (H302) Acute Tox. 4 (H312) Acute Tox. 4 (H332)

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Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

Eye Contact	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.
Skin Contact	Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.
Ingestion	Do NOT induce vomiting. Call a physician or poison control center immediately.
Inhalation	Remove to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.
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.

4.2. Most important symptoms and effects, both acute and delayed

No information available.

4.3. Indication of any immediate medical attention and special treatment needed

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Water spray, carbon dioxide (CO₂), dry chemical, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

No information available.

5.2. Special hazards arising from the substance or mixture

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

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂), Nitrogen oxides (NO_x), Bromine, Hydrogen halides.

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

SECTION 6: ACCIDENTAL RELEASE MEASURES

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6.1. Personal precautions, protective equipment and emergency procedures

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

6.2. Environmental precautions

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

6.3. Methods and material for containment and cleaning up

Sweep up and shovel into suitable containers for disposal. Avoid dust formation.

6.4. Reference to other sections

Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Avoid dust formation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

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

Technical Rules for Hazardous Substances (TRGS) 510 Class 11
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

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No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

Engineering Measures

Use only under a chemical fume hood. 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 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
Disposable gloves	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

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.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use In case of insufficient ventilation, wear suitable respiratory equipment

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

Environmental exposure controls No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State Solid

Appearance Off-white

Odor No information available

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Odor Threshold	No data available	
Melting Point/Range	120 - 121 °C / 248 - 249.8 °F	
Softening Point	No data available	
Boiling Point/Range	No information available	
Flammability (liquid)	Not applicable	Solid
Flammability (solid,gas)	No information available	
Explosion Limits	No data available	
Flash Point	No data available	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	No information available	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	No data available	
Bulk Density	No data available	
Vapor Density	No data available	(Air = 1.0)
Particle characteristics	No data available	

9.2. Other information

Molecular Formula	C8 H6 Br N O
Molecular Weight	212.05

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity
None known, based on information available

10.2. Chemical stability
Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous Polymerization Hazardous polymerization does not occur.
Hazardous Reactions None under normal processing.

10.4. Conditions to avoid
Incompatible products. Excess heat. Avoid dust formation.

10.5. Incompatible materials
Strong oxidizing agents. Strong acids. Strong bases.

10.6. Hazardous decomposition products
Carbon monoxide (CO). Carbon dioxide (CO₂). Nitrogen oxides (NO_x). Bromine. Hydrogen halides.

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information No acute toxicity information is available for this product

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(a) acute toxicity;	
Oral	No data available
Dermal	No data available
Inhalation	No data available
(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
Results / Target organs	Respiratory system.
(i) STOT-repeated exposure;	No data available
Target Organs	No information available.
(j) aspiration hazard;	No data available
Symptoms / effects,both acute and delayed	No information available.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

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

12.2. Persistence and degradability No information available

12.3. Bioaccumulative potential No information available

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12.4. Mobility in soil	No information available
12.5. Results of PBT and vPvB assessment	No data available for assessment.
12.6. Endocrine disrupting properties Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
12.7. Other adverse effects Persistent Organic Pollutant Ozone Depletion Potential	This product does not contain any known or suspected substance This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

Waste from Residues/Unused Products	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
Contaminated Packaging	Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.
European Waste Catalogue (EWC)	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
Other Information	Waste codes should be assigned by the user based on the application for which the product was used.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number	UN3439
14.2. UN proper shipping name Technical Shipping Name	NITRILES, SOLID, TOXIC, N.O.S. 3-Bromo-4-methoxybenzonitrile
14.3. Transport hazard class(es)	6.1
14.4. Packing group	III

ADR

14.1. UN number	UN3439
14.2. UN proper shipping name Technical Shipping Name	NITRILES, SOLID, TOXIC, N.O.S. 3-Bromo-4-methoxybenzonitrile
14.3. Transport hazard class(es)	6.1
14.4. Packing group	III

IATA

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14.1. UN number	UN3439
14.2. UN proper shipping name	NITRILES, SOLID, TOXIC, N.O.S.
Technical Shipping Name	3-Bromo-4-methoxybenzotrile
14.3. Transport hazard class(es)	6.1
14.4. Packing group	III
14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required.
14.7. Maritime transport in bulk according to IMO instruments	Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
3-Bromo-4-methoxybenzotrile	117572-79-9	-	-	-	-	X	-	-	-

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
3-Bromo-4-methoxybenzotrile	117572-79-9	-	-	-	-	-	-	-

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
3-Bromo-4-methoxybenzotrile	117572-79-9	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
3-Bromo-4-methoxybenzotrile	117572-79-9	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at

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work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification Water endangering class = 3 (self classification)

15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

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/NDSL - 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 Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

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

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

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

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

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

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

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Creation Date 30-Apr-2010

Revision Date 11-Oct-2023

Revision Summary Not applicable.

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This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

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