



SAFETY DATA SHEET

4-Bromo-3-cyanoanisole

According to Regulation (EC) No 1907/2006, Annex II, as amended. Commission Regulation (EU) No 2015/830 of 28 May 2015.

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

1.1. Product identifier

Product name	4-Bromo-3-cyanoanisole
Product number	FB55427
Synonyms; trade names	2-Bromo-5-methoxybenzonitrile
CAS number	138642-47-4

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

Identified uses	Laboratory reagent. Manufacture of substances. Research and development.
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1.3. Details of the supplier of the safety data sheet

Supplier	Carbosynth Ltd 8&9 Old Station Business Park Compton Berkshire RG20 6NE UK +44 1635 578444 +44 1635 579444 info@carbosynth.com
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1.4. Emergency telephone number

Emergency telephone	+44 7887 998634
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SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

Classification (EC 1272/2008)

Physical hazards	Not Classified
Health hazards	Acute Tox. 4 - H302 Eye Irrit. 2 - H319
Environmental hazards	Not Classified

2.2. Label elements

Pictogram



Signal word	Warning
Hazard statements	H302 Harmful if swallowed. H319 Causes serious eye irritation.

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Precautionary statements	P270 Do not eat, drink or smoke when using this product. P280 Wear protective gloves/ protective clothing/ eye protection/ face protection. P301+P312 IF SWALLOWED: Call a POISON CENTRE/doctor if you feel unwell. P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. P337+P313 If eye irritation persists: Get medical advice/ attention. P501 Dispose of contents/ container in accordance with national regulations.
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2.3. Other hazards

No data available.

SECTION 3: Composition/information on ingredients

3.1. Substances

Product name	4-Bromo-3-cyanoanisole
CAS number	138642-47-4
Chemical formula	C ₈ H ₆ BrNO

SECTION 4: First aid measures

4.1. Description of first aid measures

General information	Get medical advice/attention if you feel unwell.
Inhalation	Remove person to fresh air and keep comfortable for breathing. If breathing stops, provide artificial respiration. When breathing is difficult, properly trained personnel may assist affected person by administering oxygen. Get medical attention if symptoms are severe or persist.
Ingestion	Do not induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth thoroughly with water. Give plenty of water to drink. Get medical attention if symptoms are severe or persist.
Skin contact	Remove contaminated clothing. Rinse with water. Continue to rinse for at least 15 minutes. Wash contaminated clothing before reuse. Get medical attention if symptoms are severe or persist.
Eye contact	Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes. Get medical attention if symptoms are severe or persist.

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

General information	See Section 11 for additional information on health hazards.
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4.3. Indication of any immediate medical attention and special treatment needed

Notes for the doctor	Treat symptomatically.
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SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media	Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire.
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5.2. Special hazards arising from the substance or mixture

Specific hazards	None known.
Hazardous combustion products	Thermal decomposition or combustion products may include the following substances: Oxides of carbon. Oxides of nitrogen. Hydrogen bromide (HBr).

5.3. Advice for firefighters

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Special protective equipment for firefighters Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing conforming to European standard EN469 (including helmets, protective boots and gloves) will provide a basic level of protection for chemical incidents. Use protective equipment appropriate for surrounding materials.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of dust and vapours. Provide adequate ventilation.

6.2. Environmental precautions

Environmental precautions Avoid discharge into drains or watercourses or onto the ground.

6.3. Methods and material for containment and cleaning up

Methods for cleaning up Wear protective clothing as described in Section 8 of this safety data sheet. Collect powder using special dust vacuum cleaner with particle filter or carefully sweep into suitable waste disposal containers and seal securely. Clear up spills immediately and dispose of waste safely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. For waste disposal, see Section 13.

6.4. Reference to other sections

Reference to other sections For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Usage precautions Wear protective clothing as described in Section 8 of this safety data sheet. Wash hands thoroughly after handling. Provide adequate ventilation. Avoid generation and spreading of dust. Avoid contact with skin and eyes. Avoid inhalation of dust and vapours.

7.2. Conditions for safe storage, including any incompatibilities

Storage precautions Keep container tightly closed. Store contents under inert gas. Store at room temperature.

7.3. Specific end use(s)

Specific end use(s) The identified uses for this product are detailed in Section 1.2.

SECTION 8: Exposure Controls/personal protection

8.1. Control parameters

Occupational exposure limits

No exposure limits known for ingredient(s).

8.2. Exposure controls

Appropriate engineering controls Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

Eye/face protection Unless the assessment indicates a higher degree of protection is required, the following protection should be worn: Tight-fitting safety glasses. Personal protective equipment for eye and face protection should comply with European Standard EN166.

Hand protection Wear protective gloves. To protect hands from chemicals, gloves should comply with European Standard EN374.

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Other skin and body protection Wear appropriate clothing to prevent repeated or prolonged skin contact.

Respiratory protection Respiratory protection complying with an approved standard should be worn if a risk assessment indicates inhalation of contaminants is possible. Ensure all respiratory protective equipment is suitable for its intended use and is 'CE'-marked. Particulate filters should comply with European Standard EN143. Full face mask respirators with replaceable filter cartridges should comply with European Standard EN136. Half mask and quarter mask respirators with replaceable filter cartridges should comply with European Standard EN140.

Environmental exposure controls Keep container tightly sealed when not in use.

SECTION 9: Physical and Chemical Properties

9.1. Information on basic physical and chemical properties

Appearance	Solid.
Odour	No data available.
Odour threshold	No data available.
pH	No data available.
Melting point	99 to 102°C
Initial boiling point and range	No data available.
Flash point	No data available.
Evaporation rate	No data available.
Flammability (solid, gas)	No data available.
Upper/lower flammability or explosive limits	No data available.
Vapour pressure	No data available.
Vapour density	No data available.
Relative density	No data available.
Solubility(ies)	No data available.
Partition coefficient	log Pow: 2.249
Auto-ignition temperature	No data available.
Decomposition Temperature	No data available.
Viscosity	No data available.
Explosive properties	No data available.
Oxidising properties	No data available.

9.2. Other information

Molecular weight 212.04

SECTION 10: Stability and reactivity

10.1. Reactivity

Reactivity No data available.

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10.2. Chemical stability

Stability Stable under the prescribed storage conditions.

10.3. Possibility of hazardous reactions

Possibility of hazardous reactions No data available.

10.4. Conditions to avoid

Conditions to avoid No data available.

10.5. Incompatible materials

Materials to avoid Strong oxidising agents.

10.6. Hazardous decomposition products

Hazardous decomposition products Oxides of carbon. Oxides of nitrogen. Hydrogen bromide (HBr).

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity - oral

Notes (oral LD₅₀) Acute Tox. 4 - H302 Harmful if swallowed.

ATE oral (mg/kg) 500.0

Acute toxicity - dermal

Notes (dermal LD₅₀) Based on available data the classification criteria are not met.

Acute toxicity - inhalation

Notes (inhalation LC₅₀) Based on available data the classification criteria are not met.

Skin corrosion/irritation

Animal data Based on available data the classification criteria are not met.

Serious eye damage/irritation

Serious eye damage/irritation Causes serious eye irritation.

Respiratory sensitisation

Respiratory sensitisation Based on available data the classification criteria are not met.

Skin sensitisation

Skin sensitisation Based on available data the classification criteria are not met.

Germ cell mutagenicity

Genotoxicity - in vitro Based on available data the classification criteria are not met.

Carcinogenicity

Carcinogenicity Based on available data the classification criteria are not met.

IARC carcinogenicity

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.

Reproductive toxicity

Reproductive toxicity - fertility Based on available data the classification criteria are not met.

Reproductive toxicity - development

Based on available data the classification criteria are not met.

Specific target organ toxicity - single exposure

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STOT - single exposure Not classified as a specific target organ toxicant after a single exposure.

Specific target organ toxicity - repeated exposure

STOT - repeated exposure Not classified as a specific target organ toxicant after repeated exposure.

Aspiration hazard

Aspiration hazard Not relevant. Solid.

General information

Dust may irritate the eyes and the respiratory system. The severity of the symptoms described will vary dependent on the concentration and the length of exposure.

Inhalation

Dust may irritate the respiratory system. Frequent inhalation of dust over a long period of time increases the risk of developing lung diseases.

Ingestion

May cause discomfort if swallowed. Stomach pain. Nausea, vomiting.

Skin contact

Prolonged contact may cause dryness of the skin.

Eye contact

Irritating to eyes.

Route of exposure

Ingestion Inhalation Skin and/or eye contact

Target organs

No specific target organs known.

SECTION 12: Ecological Information

Ecotoxicity

Not regarded as dangerous for the environment. However, large or frequent spills may have hazardous effects on the environment.

12.1. Toxicity

Toxicity

Based on available data the classification criteria are not met.

12.2. Persistence and degradability

Persistence and degradability

The degradability of the product is not known.

12.3. Bioaccumulative potential

Bioaccumulative potential

No data available on bioaccumulation.

Partition coefficient

log Pow: 2.249

12.4. Mobility in soil

Mobility

No data available.

12.5. Results of PBT and vPvB assessment

Results of PBT and vPvB assessment

No data available.

12.6. Other adverse effects

Other adverse effects

None known.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

General information

Dispose of waste to licensed waste disposal site in accordance with the requirements of the local Waste Disposal Authority. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered.

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Disposal methods Mix or dissolve the material in a combustible solvent and burn in chemical incinerator equipped with an afterburner and scrubber.

SECTION 14: Transport information

General The product is not covered by international regulations on the transport of dangerous goods (IMDG, IATA, ADR/RID).

14.1. UN number

Not applicable.

14.2. UN proper shipping name

Not applicable.

14.3. Transport hazard class(es)

No transport warning sign required.

14.4. Packing group

Not applicable.

14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

14.6. Special precautions for user

Not applicable.

14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Not applicable.

**Annex II of MARPOL 73/78
and the IBC Code**

SECTION 15: Regulatory information

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

National regulations

Health and Safety at Work etc. Act 1974 (as amended).
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].
EH40/2005 Workplace exposure limits.

EU legislation

Regulation (EC) No 1907/2006 of the European Parliament and of the Council of 18 December 2006 concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) (as amended).
Commission Regulation (EU) No 2015/830 of 28 May 2015.
Regulation (EC) No 1272/2008 of the European Parliament and of the Council of 16 December 2008 on classification, labelling and packaging of substances and mixtures (as amended).

15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

SECTION 16: Other information

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Abbreviations and acronyms used in the safety data sheet	ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road. ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways. RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail. IATA: International Air Transport Association. ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air. IMDG: International Maritime Dangerous Goods. CAS: Chemical Abstracts Service. ATE: Acute Toxicity Estimate. LC ₅₀ : Lethal Concentration to 50 % of a test population. LD ₅₀ : Lethal Dose to 50% of a test population (Median Lethal Dose). EC ₅₀ : 50% of maximal Effective Concentration. PBT: Persistent, Bioaccumulative and Toxic substance. vPvB: Very Persistent and Very Bioaccumulative.
Training advice	Only trained personnel should use this material.
Revision date	31/01/2018
Revision	1
SDS number	144926
Hazard statements in full	H302 Harmful if swallowed. H319 Causes serious eye irritation.

This 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. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.