

SAFETY DATA SHEET
3-BROMO-4-METHYLBENZONITRILE

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Compilation date: 18/12/2006
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Revision No: 3

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

1.1. Product identifier

Product name: 3-BROMO-4-METHYLBENZONITRILE
CAS number: 42872-74-2
Product code: OR3157
Synonyms: 2-BROMO-4-CYANOTOLUENE
3-BROMO-P-TOLUNITRILE

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

1.3. Details of the supplier of the safety data sheet

Company name: Apollo Scientific Ltd
Units 3 & 4
Parkway
Denton
Manchester
M34 3SG
UK
Tel: 0161 337 9971
Fax: 0161 336 6932
Email: david.tideswell@apolloscientific.co.uk

1.4. Emergency telephone number

Section 2: Hazards identification

2.1. Classification of the substance or mixture

Classification under CLP: Acute Tox. 4: H302+312+332; Skin Irrit. 2: H315; Eye Irrit. 2: H319; STOT SE 3: H335

Classification under CHIP: Xn: R20/21/22; Xi: R36/37/38

Most important adverse effects: Harmful if swallowed, in contact with skin or if inhaled. Causes skin irritation. Causes serious eye irritation. May cause respiratory irritation.

2.2. Label elements

Label elements:

Hazard statements: H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H335: May cause respiratory irritation.

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Signal words: Warning

Hazard pictograms: GHS07: Exclamation mark



Precautionary statements: P261: Avoid breathing dust.

P271: Use only outdoors or in a well-ventilated area.

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

2.3. Other hazards

PBT: This product is not identified as a PBT/vPvB substance.

Section 3: Composition/information on ingredients

3.1. Substances

Chemical identity: 3-BROMO-4-METHYLBENZONITRILE

CAS number: 42872-74-2

Section 4: First aid measures

4.1. Description of first aid measures

Skin contact: Remove all contaminated clothes and footwear immediately unless stuck to skin.

Drench the affected skin with running water for 10 minutes or longer if substance is still on skin. Consult a doctor.

Eye contact: Bathe the eye with running water for 15 minutes. Consult a doctor.

Ingestion: Wash out mouth with water. Do not induce vomiting. If conscious, give half a litre of water to drink immediately. Consult a doctor.

Inhalation: Remove casualty from exposure ensuring one's own safety whilst doing so. Consult a doctor.

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

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

Delayed / immediate effects: No data available.

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

Section 5: Fire-fighting measures

5.1. Extinguishing media

Extinguishing media: Suitable extinguishing media for the surrounding fire should be used. Carbon dioxide. Dry chemical powder.

[cont...]

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5.2. Special hazards arising from the substance or mixture

Exposure hazards: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NOx). Hydrogen bromide (HBr). Hydrogen cyanide (HCN).

5.3. Advice for fire-fighters

Advice for fire-fighters: Wear self-contained breathing apparatus. Wear protective clothing to prevent contact with skin and eyes.

Section 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

Personal precautions: Refer to section 8 of SDS for personal protection details. If outside do not approach from downwind. If outside keep bystanders upwind and away from danger point. Mark out the contaminated area with signs and prevent access to unauthorised personnel.

6.2. Environmental precautions

Environmental precautions: Do not discharge into drains or rivers.

6.3. Methods and material for containment and cleaning up

Clean-up procedures: Transfer to a closable, labelled salvage container for disposal by an appropriate method.

6.4. Reference to other sections

Section 7: Handling and storage

7.1. Precautions for safe handling

Handling requirements: Avoid direct contact with the substance. Ensure there is sufficient ventilation of the area. Do not handle in a confined space. Avoid the formation or spread of dust in the air. Only use in fume hood.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions: Store in a cool, well ventilated area. Keep container tightly closed. Light Sensitive.

Suitable packaging: Must only be kept in original packaging.

7.3. Specific end use(s)

Specific end use(s): No special requirement.

Section 8: Exposure controls/personal protection

8.1. Control parameters

Workplace exposure limits: No data available.

DNEL/PNEC Values

DNEL / PNEC No data available.

[cont...]

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8.2. Exposure controls

Engineering measures: Ensure there is sufficient ventilation of the area.

Respiratory protection: Self-contained breathing apparatus must be available in case of emergency. Respiratory protective device with particle filter.

Hand protection: Protective gloves.

Eye protection: Safety glasses. Ensure eye bath is to hand.

Skin protection: Protective clothing.

Section 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

State: Solid

Colour: Cream

Solubility in water: Insoluble

Melting point/range °C: 41-45

Flash point °C: >110

Part.coeff. n-octanol/water: logPow:2.873

9.2. Other information

Other information: No data available.

Section 10: Stability and reactivity

10.1. Reactivity

Reactivity: Stable under recommended transport or storage conditions.

10.2. Chemical stability

Chemical stability: Stable under normal conditions.

10.3. Possibility of hazardous reactions

Hazardous reactions: Hazardous reactions will not occur under normal transport or storage conditions.

10.4. Conditions to avoid

Conditions to avoid: Heat. Light.

10.5. Incompatible materials

Materials to avoid: Strong oxidising agents.

10.6. Hazardous decomposition products

Haz. decomp. products: In combustion emits toxic fumes of carbon dioxide / carbon monoxide. Nitrogen oxides (NO_x). Hydrogen bromide gas (HBr). Hydrogen cyanide (HCN).

Section 11: Toxicological information

11.1. Information on toxicological effects

[cont...]

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Relevant hazards for substance:

| Hazard | Route | Basis |
|-------------------------------|-------------|--------------------|
| Acute toxicity (ac. tox. 4) | INH DRM ING | Based on test data |
| Skin corrosion/irritation | DRM | Based on test data |
| Serious eye damage/irritation | OPT | Based on test data |
| STOT-single exposure | INH | Based on test data |

Symptoms / routes of exposure

Skin contact: There may be irritation and redness at the site of contact.

Eye contact: There may be irritation and redness. The eyes may water profusely.

Ingestion: There may be soreness and redness of the mouth and throat. Nausea and stomach pain may occur. There may be vomiting.

Inhalation: There may be irritation of the throat with a feeling of tightness in the chest.

Delayed / immediate effects: No data available.

Other information: Not applicable.

Section 12: Ecological information

12.1. Toxicity

Ecotoxicity values: No data available.

12.2. Persistence and degradability

Persistence and degradability: No data available.

12.3. Bioaccumulative potential

Bioaccumulative potential: No data available.

12.4. Mobility in soil

Mobility: Data not yet known

12.5. Results of PBT and vPvB assessment

PBT identification: This product is not identified as a PBT/vPvB substance.

12.6. Other adverse effects

Other adverse effects: Data not known

Section 13: Disposal considerations

13.1. Waste treatment methods

Disposal operations: Transfer to a suitable container and arrange for collection by specialised disposal company. MATERIAL SHOULD BE DISPOSED OF IN ACCORDANCE WITH LOCAL, STATE AND FEDERAL REGULATIONS

Disposal of packaging: Dispose of as special waste in compliance with local and national regulations Observe all federal, state and local environmental regulations.

[cont...]

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NB: The user's attention is drawn to the possible existence of regional or national regulations regarding disposal.

Section 14: Transport information

14.1. UN number

UN number: UN3439

14.2. UN proper shipping name

Shipping name: NITRILES, SOLID, TOXIC, N.O.S.
(3-Bromo-4-methylbenzotrile)

14.3. Transport hazard class(es)

Transport class: 6.1

14.4. Packing group

Packing group: III

14.5. Environmental hazards

Environmentally hazardous: No

Marine pollutant: No

14.6. Special precautions for user

Tunnel code: E

Transport category: 2

Section 15: Regulatory information

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

15.2. Chemical Safety Assessment

Chemical safety assessment: A chemical safety assessment has not been carried out for the substance or the mixture by the supplier.

Section 16: Other information

Other information

Other information: This safety data sheet is prepared in accordance with Commission Regulation (EU) No 453/2010.

* indicates text in the SDS which has changed since the last revision.

* Data predicted using computational software. Toxtree - Toxic Hazard Estimation by decision tree approach. [http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?](http://ecb.jrc.ec.europa.eu/qsar/qsar-tools/index.php?c=TOXTREE)
c=TOXTREE

References for toxicity data: (1) Toxicol Lett. 2006 Jul 14;164(3):221-30 ; PMID: 16464542 (2) EHP, Environmental Health Perspectives. Vol. 4, Pg. 87, 1973.

~ Data predicted using computational software ACD/ToxSuite v 2.95.1 Copyright 1994-

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Phrases used in s.2 and s.3: H302+312+332: Harmful if swallowed, in contact with skin or if inhaled.
H315: Causes skin irritation.
H319: Causes serious eye irritation.
H335: May cause respiratory irritation.
R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.
R36/37/38: Irritating to eyes, respiratory system and skin.

Legend to abbreviations: PNEC = predicted no effect level
DNEL = derived no effect level
LD50 = median lethal dose
LC50 = median lethal concentration
EC50 = median effective concentration
IC50 = median inhibitory concentration
dw = dry weight
bw = body weight
cc = closed cup
oc = open cup
MUS = mouse
GPG = guinea pig
RBT = rabbit
HAM = hamster
HMN = human
MAM = mammal
PGN = pigeon
IVN = intravenous
SCU = subcutaneous
SKN = skin
DRM = dermal
OCC = ocular/corneal
PCP = physico-chemical properties

Legal disclaimer: The material is intended for research purposes only and should be handled exclusively by those who have been fully trained in safety, laboratory and chemical handling procedures. The above information is believed to be correct to the best of our knowledge. The above information is believed to be correct to the best of our knowledge at the date of its publication, but should not be considered to be all inclusive. It should be used only as a guide for safe handling, storage, transportation and disposal. We cannot guarantee that the hazards detailed in this document are the only hazards that exist for this product. This is not a warranty and Apollo Scientific Ltd shall not be held

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liable for any damage resulting from handling or from contact with the above product.