

Safety data sheet

according to 1907/2006/EC, Article 31

Revision: 28.02.2007

Printing date 02.07.2013

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifier**

Trade name

3-Bromo-4-isopropoxy-5-methoxybenzonitrile

Stock number:

H50615

CAS Number:

515848-62-1

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

Identified use:

SU24 Scientific research and development

1.3 Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar GmbH & Co.KG
A Johnson Matthey Company
Zeppelinstr. 7b
76185 Karlsruhe / Germany
Tel: +49 (0) 721 84007 280
Fax: +49 (0) 721 84007 300
Email: tech@alfa.com
www.alfa.com

Informing department:

Product safety Tel + +049 (0) 7275 988687-0

1.4 Emergency telephone number:

Carechem 24: +44 (0) 1235 239 670 (Multi-language emergency number)

Poison Information Center Mainz

www.giftinfo.uni-mainz.de Telephone: +49(0)6131/19240

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture**

Classification according to Regulation (EC) No 1272/2008



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Acute Tox. 4 H332 Harmful if inhaled.

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2 H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

Classification according to Directive 67/548/EEC or Directive 1999/45/EC

Xn; Harmful

R20/21/22: Harmful by inhalation, in contact with skin and if swallowed.

Xi; Irritant

R36/37/38: Irritating to eyes, respiratory system and skin.

Information concerning particular hazards for human and environment:

Not applicable

Other hazards that do not result in classification

No information known.

2.2 Label elements**Labelling according to Regulation (EC) No 1272/2008**

Hazard pictograms

Signal word

Hazard statements

The substance is classified and labelled according to the CLP regulation.

GHS07

Warning

H302 Harmful if swallowed.

H312 Harmful in contact with skin.

H332 Harmful if inhaled.

H315 Causes skin irritation.

H319 Causes serious eye irritation.

H335 May cause respiratory irritation.

Precautionary statements

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

IF ON SKIN: Wash with plenty of soap and water.

P302+P352 Specific treatment (see on this label).

P321

P405

P501

Dispose of contents/container in accordance with local/regional/national/international regulations.

2.3 Other hazards

Results of PBT and vPvB assessment

PBT:

Not applicable.

vPvB:

Not applicable.

SECTION 3: Composition/information on ingredients**3.1 Substances**

CAS# Designation:

515848-62-1 3-Bromo-4-isopropoxy-5-methoxybenzonitrile

SECTION 4: First aid measures**4.1 Description of first aid measures**

After inhalation

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

After skin contact

Seek immediate medical advice.

Instantly wash with water and soap and rinse thoroughly.

After eye contact

Seek immediate medical advice.

Rinse opened eye for several minutes under running water. Then consult doctor.

After swallowing

Seek medical treatment.

4.2 Most important symptoms and effects, both acute and delayed

No further relevant information available.

4.3 Indication of any immediate medical attention and special treatment needed

No further relevant information available.

SECTION 5: Firefighting measures**5.1 Extinguishing media**

Suitable extinguishing agents

CO2, extinguishing powder or water jet. Fight larger fires with water jet or alcohol-resistant foam.

5.2 Special hazards arising from the substance or mixture

If this product is involved in a fire, the following can be released:

Carbon monoxide and carbon dioxide

Nitrogen oxides (NOx)

Hydrogen bromide (HBr)

Hydrogen cyanide (HCN)

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5.3 Advice for firefighters

Protective equipment:

Wear self-contained breathing apparatus.
Wear full protective suit.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation

6.2 Environmental precautions:

Do not allow material to be released to the environment without proper governmental permits.
Do not allow product to reach sewage system or water bodies.
Do not allow to enter the ground/soil.

6.3 Methods and material for containment and cleaning up:

Dispose of contaminated material as waste according to item 13.
Ensure adequate ventilation.

Prevention of secondary hazards:

No special measures required.

6.4 Reference to other sections

See Section 7 for information on safe handling
See section 8 for information on personal protection equipment.
See Section 13 for information on disposal.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Keep containers tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation/exhaustion at the workplace.

Information about protection against explosions and fires:

No information known.

7.2 Conditions for safe storage, including any incompatibilities

Storage Requirements to be met by storerooms and containers:

No special requirements.

Information about storage in one common storage facility:

Store away from oxidizing agents.

Further information about storage conditions:

Keep container tightly sealed.
Store in cool, dry conditions in well sealed containers.

7.3 Specific end use(s)

No further relevant information available.

SECTION 8: Exposure controls/personal protection

Additional information about design of technical systems:

Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

8.1 Control parameters

Components with critical values that require monitoring at the workplace:

Not required.

Additional information:

No data

8.2 Exposure controls

Personal protective equipment

General protective and hygienic measures

The usual precautionary measures should be adhered to in handling the chemicals.
Keep away from foodstuffs, beverages and food.
Instantly remove any soiled and impregnated garments.
Wash hands during breaks and at the end of the work.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.

Breathing equipment:

Use breathing protection with high concentrations.

Protection of hands:

Check protective gloves prior to each use for their proper condition.
The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer.

Material of gloves

Impervious gloves

Penetration time of glove material

Not determined

Eye protection:

Safety glasses

Body protection:

Face protection
Protective work clothing.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

General Information

Appearance:

Form: Powder

Smell: Not determined

Odour threshold: Not determined.

pH-value: Not applicable.

Change in condition

Melting point/Melting range: Not determined

Boiling point/Boiling range: Not determined

Sublimation temperature / start: Not determined

Flash point: Not applicable

Inflammability (solid, gaseous): Not determined.

Ignition temperature: Not determined

Decomposition temperature: Not determined

Self-inflammability: Not determined.

Danger of explosion: Product is not explosive.

Critical values for explosion:

Lower: Not determined

Upper: Not determined

Steam pressure: Not applicable.

Density: Not determined

Relative density: Not determined.

Vapour density: Not applicable.

Evaporation rate: Not applicable.

Solubility in / Miscibility with

Water: Not determined

Partition coefficient (n-octanol/water): Not determined.

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Viscosity:
dynamic: Not applicable.
kinematic: Not applicable.
9.2 Other information No further relevant information available.

SECTION 10: Stability and reactivity

10.1 Reactivity No information known.
10.2 Chemical stability Stable under recommended storage conditions.
Thermal decomposition / conditions to be avoided: No decomposition if used and stored according to specifications.
10.3 Possibility of hazardous reactions No dangerous reactions known
10.5 Incompatible materials: Oxidizing agents
10.6 Hazardous decomposition products: Carbon monoxide and carbon dioxide
 Nitrogen oxides (NOx)
 Hydrogen bromide
 Hydrogen cyanide (prussic acid)

SECTION 11: Toxicological information

11.1 Information on toxicological effects
Acute toxicity: Harmful if inhaled.
 Harmful in contact with skin.
 Harmful if swallowed.
 Danger by skin resorption.
LD/LC50 values that are relevant for classification: No data
Skin irritation or corrosion: Causes skin irritation.
Eye irritation or corrosion: Causes serious eye irritation.
Sensitization: No sensitizing effect known.
Germ cell mutagenicity: No effects known.
Carcinogenicity: No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.
Reproductive toxicity: No effects known.
Specific target organ system toxicity - repeated exposure: No effects known.
Specific target organ system toxicity - single exposure: May cause respiratory irritation.
Aspiration hazard: No effects known.
Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

SECTION 12: Ecological information

12.1 Toxicity
Aquatic toxicity: No further relevant information available.
12.2 Persistence and degradability No further relevant information available.
12.3 Bioaccumulative potential No further relevant information available.
12.4 Mobility in soil No further relevant information available.
Additional ecological information:
General notes: Do not allow material to be released to the environment without proper governmental permits.
 Water hazard class 1 (Self-assessment): slightly hazardous for water.
 Do not allow undiluted product or large quantities of it to reach ground water, water bodies or sewage system.
 Avoid transfer into the environment.
12.5 Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
12.6 Other adverse effects No further relevant information available.

SECTION 13: Disposal considerations

13.1 Waste treatment methods
Recommendation Hand over to disposers of hazardous waste.
 Must be specially treated under adherence to official regulations.
 Consult state, local or national regulations for proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

SECTION 14: Transport information

UN-Number
ADR, IMDG, IATA UN3439
14.2 UN proper shipping name
ADR 3439 NITRILES, TOXIC, SOLID, N.O.S. (3-Bromo-4-isopropoxy-5-methoxybenzonitrile)
IMDG, IATA NITRILES, TOXIC, SOLID, N.O.S. (3-Bromo-4-isopropoxy-5-methoxybenzonitrile)
14.3 Transport hazard class(es)
ADR

Class 6.1 (T2) Toxic substances.
Label 6.1
IMDG, IATA

Class 6.1 Toxic substances.
Label 6.1
Packing group
ADR, IMDG, IATA III
14.5 Environmental hazards: Not applicable.

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14.6 Special precautions for user

Kemler Number:

Warning: Toxic substances.
60**14.7 Transport in bulk according to Annex II of MARPOL73/78 and the IBC**

Code

Not applicable.

Transport/Additional information:

ADR

Excepted quantities (EQ):

Limited quantities (LQ)

Transport category

Tunnel restriction code

E1

5 kg

2

E

UN "Model Regulation":

UN3439, NITRILES, TOXIC, SOLID, N.O.S. (3-Bromo-4-isopropoxy-5-methoxybenzonitrile), 6.1, III

SECTION 15: Regulatory information**15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**

Australian Inventory of Chemical

Substances

Substance is not listed.

Standard for the Uniform Scheduling of

Drugs and Poisons

Substance is not listed.

National regulations

Information about limitation of use:

For use only by technically qualified individuals.

Employment restrictions concerning young persons must be observed.

Water hazard class:

Water hazard class 1 (Self-assessment): slightly hazardous for water.

Other regulations, limitations and prohibitive regulations

ELINCS (European List of Notified Chemical

Substances)

Substance is not listed.

Substances of very high concern (SVHC)

according to REACH, Article 57

REACH - Pre-registered substances

Substance is not listed.

Substance is not listed.

15.2 Chemical safety assessment:

A Chemical Safety Assessment has not been carried out.

SECTION 16: Other information

Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing data specification sheet: Health, Safety and Environmental Department.**Abbreviations and acronyms:**

ADR: Accord européen sur le transport des marchandises dangereuses par Route (European Agreement concerning the International Carriage of Dangerous Goods by Road)

IMDG: International Maritime Code for Dangerous Goods

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

CAS: Chemical Abstracts Service (division of the American Chemical Society)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

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