

1 Identification

Product identifier

Product name: 3-Bromo-4-fluorobenzonitrile

Stock number: A13318, L13475

CAS Number:

79630-23-2

EC number:

279-200-7

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

Identified use: SU24 Scientific research and development

Details of the supplier of the safety data sheet

Manufacturer/Supplier:

Alfa Aesar

Thermo Fisher Scientific Chemicals, Inc.

30 Bond Street

Ward Hill, MA 01835-8099

Tel: 800-343-0660

Fax: 800-322-4757

Email: tech@alfa.com

www.alfa.com

Information Department: Health, Safety and Environmental Department

Emergency telephone number:

During normal business hours (Monday-Friday, 8am-7pm EST), call (800) 343-0660. After normal business hours, call Carechem 24 at (866) 928-0789.

2 Hazard(s) identification

Classification of the substance or mixture in accordance with 29 CFR 1910 (OSHA HCS)



GHS06 Skull and crossbones

Acute Tox. 3 H331 Toxic if inhaled.



GHS07

Acute Tox. 4 H302 Harmful if swallowed.

Acute Tox. 4 H312 Harmful in contact with skin.

Skin Irrit. 2 H315 Causes skin irritation.

Eye Irrit. 2A H319 Causes serious eye irritation.

STOT SE 3 H335 May cause respiratory irritation.

Hazards not otherwise classified No information known.

Label elements

GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)

Hazard pictograms



GHS06

Signal word

Danger

Hazard statements

H302+H312 Harmful if swallowed or in contact with skin.

H331 Toxic 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/vapors/spray

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.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P405 Store locked up.

P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

WHMIS classification

D1B - Toxic material causing immediate and serious toxic effects

D2B - Toxic material causing other toxic effects



Classification system

HMIS ratings (scale 0-4)

(Hazardous Materials Identification System)

HEALTH 2 Health (acute effects) = 2

FIRE 1 Flammability = 1

REACTIVITY 1 Physical Hazard = 1

Other hazards

Results of PBT and vPvB assessment

PBT: Not applicable.

vPvB: Not applicable.

3 Composition/information on ingredients

Chemical characterization: Substances

CAS# Description:

79630-23-2 3-Bromo-4-fluorobenzonitrile

Product name: 3-Bromo-4-fluorobenzonitrile

Concentration: ≤100%
Identification number(s):
EC number: 279-200-7

(Contd. of page 1)

4 First-aid measures

Description of first aid measures
After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Seek medical treatment.
Information for doctor
Most important symptoms and effects, both acute and delayed
Causes skin irritation.
Harmful if swallowed.
Causes serious eye irritation.
Harmful in contact with skin.
Toxic if inhaled.
Indication of any immediate medical attention and special treatment needed No further relevant information available.

5 Fire-fighting measures

Extinguishing media
Suitable extinguishing agents Carbon dioxide, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
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
Hydrogen fluoride (HF)
Hydrogen cyanide (HCN)
Nitrogen oxides (NOx)
Hydrogen bromide (HBr)
Advice for firefighters
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Personal precautions, protective equipment and emergency procedures
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Environmental precautions: Do not allow product to reach sewage system or any water course.
Methods and material for containment and cleaning up:
Dispose of contaminated material as waste according to section 13.
Ensure adequate ventilation.
Prevention of secondary hazards: No special measures required.
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 disposal information.
Protective Action Criteria for Chemicals
PAC-1: Substance is not listed.
PAC-2: Substance is not listed.
PAC-3: Substance is not listed.

7 Handling and storage

Handling
Precautions for safe handling
Keep container tightly sealed.
Store in cool, dry place in tightly closed containers.
Ensure good ventilation at the workplace.
Information about protection against explosions and fires: No information known.
Conditions for safe storage, including any incompatibilities
Storage
Requirements to be met by storerooms and receptacles: 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.
Specific end use(s) No further relevant information available.

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.
Control parameters
Components with limit values that require monitoring at the workplace:
The product does not contain any relevant quantities of materials with critical values that have to be monitored at the workplace.
Additional information: No data
Exposure controls
Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Avoid contact with the eyes and skin.
Maintain an ergonomically appropriate working environment.

(Contd. on page 3)
USA

Product name: 3-Bromo-4-fluorobenzonitrile

(Contd. of page 2)

Breathing equipment: Use suitable respirator when high concentrations are present.

Recommended filter device for short term use:

Use a respirator with type P100 (USA) or P3 (EN 143) cartridges as a backup to engineering controls. Risk assessment should be performed to determine if air-purifying respirators are appropriate. Only use equipment tested and approved under appropriate government standards.

Protection of hands:

Impervious gloves

Check protective gloves prior to each use for their proper condition.

The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.

Eye protection: Safety glasses with side shields / NIOSH (US) or EN 166(EU)

Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties

General Information

Appearance:

Form: Solid

Odor: Not determined

Odor threshold: Not determined.

pH-value: Not applicable.

Change in condition

Melting point/Melting range: 56-58 °C (133-136 °F)

Boiling point/Boiling range: 134-136 °C (273-277 °F) (33mm)

Sublimation temperature / start: Not determined

Flammability (solid, gaseous) Not determined.

Ignition temperature: Not determined

Decomposition temperature: Not determined

Auto igniting: Not determined.

Danger of explosion: Not determined.

Explosion limits:

Lower: Not determined

Upper: Not determined

Vapor pressure: Not applicable.

Density: Not determined

Relative density Not determined.

Vapor density Not applicable.

Evaporation rate Not applicable.

Solubility in / Miscibility with

Water: Not determined

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

Viscosity:

dynamic: Not applicable.

kinematic: Not applicable.

Other information No further relevant information available.

10 Stability and reactivity

Reactivity No information known.

Chemical stability Stable under recommended storage conditions.

Thermal decomposition / conditions to be avoided: Decomposition will not occur if used and stored according to specifications.

Possibility of hazardous reactions Reacts with strong oxidizing agents

Conditions to avoid No further relevant information available.

Incompatible materials: Oxidizing agents

Hazardous decomposition products:

Carbon monoxide and carbon dioxide

Hydrogen fluoride

Hydrogen cyanide

Nitrogen oxides

Hydrogen bromide

11 Toxicological information

Information on toxicological effects

Acute toxicity:

Harmful in contact with skin.

Harmful if swallowed.

Toxic if inhaled.

Danger through skin absorption.

LD/LC50 values that are relevant for classification: No data

Skin irritation or corrosion: May cause irritation

Eye irritation or corrosion: May cause irritation

Sensitization: No sensitizing effects 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.

Subacute to chronic toxicity: No effects known.

Additional toxicological information: To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.

12 Ecological information

Toxicity

Aquatic toxicity: No further relevant information available.

Persistence and degradability No further relevant information available.

Bioaccumulative potential No further relevant information available.

Mobility in soil No further relevant information available.

(Contd. on page 4)
USA

Product name: 3-Bromo-4-fluorobenzonitrile

(Contd. of page 3)

Additional ecological information:
General notes:
Do not allow undiluted product or large quantities to reach ground water, water course or sewage system.
Avoid transfer into the environment.
Results of PBT and vPvB assessment
PBT: Not applicable.
vPvB: Not applicable.
Other adverse effects No further relevant information available.

13 Disposal considerations
Waste treatment methods
Recommendation Consult state, local or national regulations to ensure proper disposal.
Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

UN-Number DOT, IMDG, IATA	UN3439
UN proper shipping name DOT ADR IMDG, IATA	Nitriles, solid, toxic, n.o.s. (3-Bromo-4-fluorobenzonitrile) 3439 Nitriles, solid, toxic, n.o.s. (3-Bromo-4-fluorobenzonitrile) NITRILES, SOLID, TOXIC, N.O.S. (3-Bromo-4-fluorobenzonitrile)
Transport hazard class(es) DOT 	6.1 Toxic substances 6.1
Class Label ADR 	6.1 (T2) Toxic substances 6.1
Class Label IMDG, IATA 	6.1 Toxic substances 6.1
Packing group DOT, ADR, IMDG, IATA	III
Environmental hazards:	Not applicable.
Special precautions for user EMS Number: Stowage Category Segregation Code	Warning: Toxic substances F-A,S-A A SG35 Stow "separated from" acids.
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information: DOT Quantity limitations Marine Pollutant (DOT):	On passenger aircraft/rail: 100 kg On cargo aircraft only: 200 kg No
IMDG Limited quantities (LQ) Excepted quantities (EQ)	5 kg Code: E1 Maximum net quantity per inner packaging: 30 g Maximum net quantity per outer packaging: 1000 g
UN "Model Regulation":	UN 3439 NITRILES, SOLID, TOXIC, N.O.S. (3-BROMO-4-FLUOROBENZONITRILE), 6.1, III

15 Regulatory information
Safety, health and environmental regulations/legislation specific for the substance or mixture
GHS label elements The product is classified and labeled in accordance with 29 CFR 1910 (OSHA HCS)
Hazard pictograms

GHS06
Signal word Danger
Hazard statements
H302+H312 Harmful if swallowed or in contact with skin.
H331 Toxic 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/vapors/spray

(Contd. on page 5)
USA

Product name: 3-Bromo-4-fluorobenzonitrile

(Contd. of page 4)

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.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P405 Store locked up.
P501 Dispose of contents/container in accordance with local/regional/national/international regulations.

National regulations

This product is not listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical Substance Inventory. Use of this product is restricted to research and development only. This product must be used by or directly under the supervision of a technically qualified individual as defined by TSCA. This product must not be used for commercial purposes or in formulations for commercial purposes.

This product is not listed on the Canadian Domestic Substances List (DSL) or the Canadian Non-Domestic Substances List (NDSL).

SARA Section 313 (specific toxic chemical listings) Substance is not listed.

California Proposition 65

Prop 65 - Chemicals known to cause cancer Substance is not listed.

Prop 65 - Developmental toxicity Substance is not listed.

Prop 65 - Developmental toxicity, female Substance is not listed.

Prop 65 - Developmental toxicity, male Substance is not listed.

Information about limitation of use: For use only by technically qualified individuals.

Other regulations, limitations and prohibitive regulations

Substance of Very High Concern (SVHC) according to the REACH Regulations (EC) No. 1907/2006. Substance is not listed.

The conditions of restrictions according to Article 67 and Annex XVII of the Regulation (EC) No 1907/2006 (REACH) for the manufacturing, placing on the market and use must be observed.

Substance is not listed.

Annex XIV of the REACH Regulations (requiring Authorisation for use) Substance is not listed.

Chemical safety assessment: A Chemical Safety Assessment has not been carried out.

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 Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing SDS: Global Marketing Department

Date of preparation/Revision: Print date, revision date and version number are in the header of each page.

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

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

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

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic

SVHC: Substances of Very High Concern

vPvB: very Persistent and very Bioaccumulative

ACGIH: American Conference of Governmental Industrial Hygienists (USA)

OSHA: Occupational Safety and Health Administration (USA)

NTP: National Toxicology Program (USA)

IARC: International Agency for Research on Cancer

EPA: Environmental Protection Agency (USA)

Acute Tox. 4: Acute toxicity – Category 4

Acute Tox. 3: Acute toxicity – Category 3

Skin Irrit. 2: Skin corrosion/irritation – Category 2

Eye Irrit. 2A: Serious eye damage/eye irritation – Category 2A

STOT SE 3: Specific target organ toxicity (single exposure) – Category 3