

1 Identification

Product identifier

Product name: **3-Bromo-5-methoxy-4-acetoxymbenzonitrile**

Stock number: H50614

CAS Number:

515847-71-9

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/vapours/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:

515847-71-9 3-Bromo-5-methoxy-4-acetoxymbenzonitrile

Product name: **3-Bromo-5-methoxy-4-acetoxybenzonitrile**

(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 No further relevant information available.
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
Nitrogen oxides (NOx)
Hydrogen bromide (HBr)
Hydrogen cyanide (HCN)
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 material to be released to the environment without proper governmental permits.
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.

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: Not required.
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.
Breathing equipment: Use suitable respirator when high concentrations are present.
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.
Penetration time of glove material (in minutes) Not determined
Eye protection: Safety glasses
Body protection: Protective work clothing.

9 Physical and chemical properties

Information on basic physical and chemical properties
General Information
Appearance:
Form: Powder

(Contd. on page 3)
USA

Product name: 3-Bromo-5-methoxy-4-acetoxybenzonitrile

(Contd. of page 2)

Odor: Not determined
Odor 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
Flammability (solid, gaseous) Not determined.
Ignition temperature: Not determined
Decomposition temperature: Not determined
Auto igniting: Not determined.

Danger of explosion: Product does not present an explosion hazard.

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 No dangerous reactions known
Conditions to avoid No further relevant information available.
Incompatible materials: Oxidizing agents
Hazardous decomposition products:
Carbon monoxide and carbon dioxide
Nitrogen oxides
Hydrogen bromide
Hydrogen cyanide

11 Toxicological information

Information on toxicological effects
Acute toxicity:
Harmful if inhaled.
Harmful in contact with skin.
Harmful if swallowed.
Danger through skin absorption.
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 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.
Subacute to chronic toxicity:
Nitriles may resemble cyanides in toxicity. Exposure to nitriles may cause increased salivation, flushing of the face, eye and respiratory tract irritation, shallow respiration, nausea, vomiting, weakness, headache and diarrhea. Jaundice, anemia, and leucocytosis has been reported in some cases.
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.
Additional ecological information:
General notes:
Do not allow material to be released to the environment without proper governmental permits.
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.

(Contd. on page 4)
USA

Product name: 3-Bromo-5-methoxy-4-acetoxybenzonitrile

Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

(Contd. of page 3)

14 Transport information

UN-Number DOT, IMDG, IATA	UN3439
UN proper shipping name DOT IMDG, IATA	Nitriles, solid, toxic, n.o.s. (3-Bromo-5-methoxy-4-acetoxybenzonitrile) NITRILES, SOLID, TOXIC, N.O.S. (3-Bromo-5-methoxy-4-acetoxybenzonitrile)
Transport hazard class(es) DOT	
	
Class Label Class Label IMDG, IATA	6.1 Toxic substances. 6.1 6.1 (T2) Toxic substances 6.1
	
Class Label	6.1 Toxic substances. 6.1
Packing group DOT, IMDG, IATA	III
Environmental hazards:	Not applicable.
Special precautions for user	Warning: Toxic substances
Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable.
Transport/Additional information:	
DOT Marine Pollutant (DOT):	No
UN "Model Regulation":	UN3439, Nitriles, solid, toxic, n.o.s. (3-Bromo-5-methoxy-4-acetoxybenzonitrile), 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/vapours/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.

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.

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 Material 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 / last revision 11/24/2015 / -

(Contd. on page 5)
USA

Product name: 3-Bromo-5-methoxy-4-acetoxybenzonitrile

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
CAS: Chemical Abstracts Service (division of the American Chemical Society)
HMS: Hazardous Materials Identification System (USA)
WHMIS: Workplace Hazardous Materials Information System (Canada)
LC50: Lethal concentration, 50 percent
LD50: Lethal dose, 50 percent
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)

(Contd. of page 4)