

SAFETY DATA SHEET

Revision Date 25-Mar-2024 Revision Number 3

1. Identification

Product Name 3-Bromophenylacetonitrile

Cat No.: B20189

CAS No 31938-07-5

Synonyms 3-Bromobenzyl cyanide

Recommended Use Laboratory chemicals.

Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc. 30 Bond Street Ward Hill. MA 01835-8099

Tel: 800-343-0660 Fax: 800-322-4757

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11 Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99 **CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity

Acute dermal toxicity

Acute Inhalation Toxicity - Dusts and Mists

Skin Corrosion/Irritation

Serious Eye Damage/Eye Irritation

Specific target organ toxicity (single exposure)

Target Organs - Respiratory system.

Label Elements

Signal Word

Warning

Hazard Statements

Causes skin irritation
Causes serious eye irritation
May cause respiratory irritation
Harmful if swallowed, in contact with skin or if inhaled



Precautionary Statements

Prevention

Wash face, hands and any exposed skin thoroughly after handling

Do not eat, drink or smoke when using this product

Wear protective gloves/protective clothing/eye protection/face protection

Avoid breathing dust/fume/gas/mist/vapors/spray

Use only outdoors or in a well-ventilated area

Inhalation

IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing

Call a POISON CENTER or doctor/physician if you feel unwell

Skin

IF ON SKIN: Wash with plenty of soap and water

Call a POISON CENTER or doctor/physician if you feel unwell

If skin irritation occurs: Get medical advice/attention

Take off contaminated clothing and wash before reuse

Eyes

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing If eye irritation persists: Get medical advice/attention

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell

Rinse mouth

Storage

Store in a well-ventilated place. Keep container tightly closed

Store locked up

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

None identified

3. Composition/Information on Ingredients

Component	CAS No	Weight %
(3-Bromophenyl)acetonitrile	31938-07-5	> 98

4. First-aid measures

Eye Contact Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get

medical attention.

Skin Contact Wash off immediately with soap and plenty of water while removing all contaminated

clothes and shoes. Get medical attention.

Inhalation Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial

respiration. Get medical attention.

Ingestion Clean mouth with water. Get medical attention.

Most important symptoms and

effects

Notes to Physician Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam.

No information available.

Unsuitable Extinguishing Media No information available

Flash Point $> 110 \, ^{\circ}\text{C} \, / > 230 \, ^{\circ}\text{F}$

Method - No information available

Autoignition Temperature

Explosion Limits

No information available

Upper No data available
Lower No data available
Sensitivity to Mechanical Impact No information available
Sensitivity to Static Discharge No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Nitrogen oxides (NOx). Carbon monoxide (CO). Carbon dioxide (CO₂). Hydrogen halides.

Protective Equipment and Precautions for Firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

NFPA

Health	Flammability	Instability	Physical hazards
2	1	0	N/A

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required.

Environmental Precautions See Section 12 for additional Ecological Information.

Methods for Containment and Clean Soak up with inert absorbent material. Sweep up and shovel into suitable containers for **Up** disposal.

Handling and storage

Handling Avoid contact with skin and eyes. Do not breathe dust.

Storage. Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Incompatible

Materials. Strong oxidizing agents. Strong bases.

8. Exposure controls / personal protection

Exposure Guidelines

Component	ACGIH TLV	OSHA PEL	NIOSH	Mexico OEL (TWA)
(3-Bromophenyl)acetonitrile		(Vacated) TWA: 5 mg/m ³	IDLH: 25 mg/m ³	

Legend

OSHA - Occupational Safety and Health Administration

NIOSH: NIOSH - National Institute for Occupational Safety and Health

Engineering Measures Ensure adequate ventilation, especially in confined areas. Ensure that eyewash stations

and safety showers are close to the workstation location.

Personal Protective Equipment

Eve/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by

OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard

EN166.

Skin and body protectionWear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard

EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Recommended Filter type: Particulates filter conforming to EN 143.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Physical State Solid

Appearance Light yellow
Odor No information available

Odor Threshold
PH
No information available
No information available
No information available

Melting Point/Range 26 - 29 °C / 78.8 - 84.2 °F

Boiling Point/Range 114 - 115 °C / 237.2 - 239 °F @ 5 mmHg

Flash Point $> 110 \, ^{\circ}\text{C} \, / > 230 \, ^{\circ}\text{F}$

Evaporation Rate Not applicable

Flammability (solid,gas) No information available

Flammability or explosive limits

UpperNo data availableLowerNo data availableVapor PressureNo information available

Vapor Density Not applicable

Specific Gravity

Solubility

Partition coefficient; n-octanol/water

No information available
No data available

Autoignition TemperatureNo information availableDecomposition TemperatureNo information available

Viscosity Not applicable
Molecular Formula C8 H6 Br N
Molecular Weight 196.05

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products.

Incompatible Materials Strong oxidizing agents, Strong bases

Hazardous Decomposition Products Nitrogen oxides (NOx), Carbon monoxide (CO), Carbon dioxide (CO2), Hydrogen halides

Hazardous Polymerization No information available.

Hazardous Reactions None under normal processing.

Toxicological information

Acute Toxicity

Product Information Component Information

Toxicologically Synergistic No information available

Products

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

Carcinogenicity The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
(3-Bromophenyl)aceto	31938-07-5	Not listed				
nitrile						

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure Respiratory system

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects,both acute and No information available

delayed

Endocrine Disruptor Information No information available

Other Adverse Effects The toxicological properties have not been fully investigated.

12. Ecological information

Ecotoxicity

Mobility

Do not empty into drains.

Persistence and Degradability No information available **Bioaccumulation/ Accumulation** No information available. No information available.

13. Disposal considerations

Waste Disposal Methods

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT

UN-No UN3449

Proper Shipping Name BROMOBENZYL CYANIDES, SOLID

Hazard Class 6.1
Packing Group

<u>TDG</u>

UN-No UN3449

Proper Shipping Name BROMOBENZYL CYANIDES, SOLID

Hazard Class 6.1 Packing Group

<u>IATA</u>

UN-No UN3449

Proper Shipping Name BROMOBENZYL CYANIDES, SOLID

Hazard Class 6.1 Packing Group

IMDG/IMO

UN-No UN3449

Proper Shipping Name BROMOBENZYL CYANIDES, SOLID

Hazard Class 6.1 Packing Group

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
(3-Bromophenyl)acetonitrile	31938-07-5	=	=	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT)

Not applicable

TSCA 12(b) - Notices of Export

Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
(3-Bromophenyl)acetonitrile	31938-07-5	-	-	250-867-6	-	-		-	-	-

KECL - NIER number or KE number (http://ncis.nier.go.kr/en/main.do)

U.S. Federal Regulations

SARA 313

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product contains a chemical or chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372.

Component	CAS No	Weight %	SARA 313 - Threshold Values %	SARA 313 - Reporting threasholds
(3-Bromophenyl)acetonitr ile	31938-07-5	> 98	1.0 %	-

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act)

	Component CWA - Hazardous Substances		CWA - Reportable Quantities	CWA - Toxic Pollutants	CWA - Priority Pollutants	
(3-B	Bromophenyl)acetonitrile	-	-	X	X	

Clean Air Act

Component	HAPS Data	Class 1 Ozone Depletors	Class 2 Ozone Depletors
(3-Bromophenyl)acetonitrile	Χ		-

OSHA - Occupational Safety and

Health Administration

Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65

This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations

Component	Massachusetts	New Jersey	Pennsylvania	Illinois	Rhode Island
(3-Bromophenyl)acetonitr	-	X	X	X	X
ile					

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant Y
DOT Severe Marine Pollutant N

U.S. Department of Homeland

Security

This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH

	Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization		REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
1	(3-Bromophenyl)acetonitrile	31938-07-5	-	-	-

Not applicable

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

Component	CAS No	OECD HPV	Persistent Organic	Ozone Depletion	Restriction of
-			Pollutant	Potential	Hazardous
					Substances (RoHS)

(3-Bromophenyl)acetonitrile	31938-07-5	Not applicable	Not applicable	Not applicable	Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)? Not applicable

Other International Regulations

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities	, ,	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
		for Major Accident	for Safety Report		
		Notification	Requirements		
(3-Bromophenyl)acetonitrile	31938-07-5	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information	
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Prepared By Health, Safety and Environmental Department

Email: chem.techinfo@thermofisher.com

www.thermofisher.com

Revision Date 25-Mar-2024 Print Date 25-Mar-2024

Revision Summary New emergency telephone response service provider.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The 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, unless specified in the text

End of SDS