

ALFAAA15460

3,5-Bis(trifluoromethyl)benzotrile

SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

产品说明: 3,5-双(三氟甲基)苯甲腈
Product Description: 3,5-Bis(trifluoromethyl)benzotrile

Cat No. : A15460
CAS No 27126-93-8
Molecular Formula C9 H3 F6 N

Supplier Avocado Research Chemicals Ltd.
(Part of Thermo Fisher Scientific)
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CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

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Recommended Use Laboratory chemicals.
Uses advised against No Information available

SECTION 2. HAZARD IDENTIFICATION

Physical State
Liquid

Appearance
Colorless

Odor
No information available

Emergency Overview

Combustible liquid. Harmful if swallowed. Harmful in contact with skin. Harmful if inhaled.

Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4

Label Elements



Signal Word

Warning

Hazard Statements

H227 - Combustible liquid

H302 + H312 + H332 - Harmful if swallowed, in contact with skin or if inhaled

Precautionary Statements**Prevention**

P280 - Wear protective gloves/protective clothing/eye protection/face protection

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

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

Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water

P312 - Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

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

P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish

P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

P403 + P235 - Store in a well-ventilated place. Keep cool

Disposal

P501 - Dispose of contents/ container to an approved waste disposal plant

Physical and Chemical Hazards

Combustible material.

Health Hazards

Harmful if swallowed. Harmful in contact with skin. Harmful if inhaled.

Environmental hazards

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants. Will likely be mobile in the environment due to its water solubility. The product is water soluble, and may spread in water systems.

This product does not contain any known or suspected endocrine disruptors.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Component	CAS No	Weight %
3,5-Bis(trifluoromethyl)benzonitrile	27126-93-8	97

SECTION 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

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

Self-Protection of the First Aider

Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

Notes to Physician

Treat symptomatically.

SECTION 5. FIRE-FIGHTING MEASURES**Suitable Extinguishing Media**

Water spray. Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers.

Extinguishing media which must not be used for safety reasons

No information available.

Specific Hazards Arising from the Chemical

Combustible material. Containers may explode when heated.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES**Personal Precautions**

Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Avoid contact with skin and eyes. Do not breathe mist/vapors/spray. Keep away from open flames, hot surfaces and sources of ignition.

Storage

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Keep containers tightly closed in a dry, cool and well-ventilated place.

Specific Use(s)

Use in laboratories

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS70 General methods for sampling airborne gases and vapours

Exposure Controls

Engineering Measures

Ensure adequate ventilation, especially in confined areas. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

Personal protective equipment

Eye Protection Goggles (European standard - EN 166)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers recommendations	-	EN 374	(minimum requirement)
Neoprene				
Natural rubber				
PVC				

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure

Respiratory Protection When workers are facing concentrations above the exposure limit they must use appropriate certified respirators. To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly

Large scale/emergency use Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced
Recommended Filter type: Organic gases and vapours filter Type A Brown conforming to EN14387

Small scale/Laboratory use Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.
Recommended half mask:- Valve filtering: EN405; or; Half mask: EN140; plus filter, EN 141
When RPE is used a face piece Fit Test should be conducted

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

Environmental exposure controls No information available.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	Colorless	
Physical State	Liquid	
Odor	No information available	
Odor Threshold	No data available	
pH	No information available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	155 °C / 311 °F	
Flash Point	72 °C / 161.6 °F	Method - No information available
Evaporation Rate	No data available	
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzotrile

Vapor Pressure	No data available	
Vapor Density	No data available	(Air = 1.0)
Specific Gravity / Density	1.420	
Bulk Density	Not applicable	Liquid
Water Solubility	soluble in most common solvents	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
Viscosity	No data available	
Explosive Properties		explosive air/vapour mixtures possible
Oxidizing Properties	No information available	
Molecular Formula	C9 H3 F6 N	
Molecular Weight	239.12	

SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	No information available.
Hazardous Polymerization	No information available.
Conditions to Avoid	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
Materials to avoid	Strong oxidizing agents. Strong acids. Strong bases. Strong reducing agents.
Hazardous Decomposition Products	Carbon monoxide (CO). Carbon dioxide (CO ₂). Gaseous hydrogen fluoride (HF).

SECTION 11. TOXICOLOGICAL INFORMATION

Product Information

(a) acute toxicity;	
(b) skin corrosion/irritation;	No data available
(c) serious eye damage/irritation;	No data available
(d) respiratory or skin sensitization;	
Respiratory	No data available
Skin	No data available
(e) germ cell mutagenicity;	No data available
(f) carcinogenicity;	No data available
	There are no known carcinogenic chemicals in this product
(g) reproductive toxicity;	No data available
(h) STOT-single exposure;	No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Contains no substances known to be hazardous to the environment or that are not degradable in waste water treatment plants.

Persistence and Degradability
Persistence Soluble in water, Persistence is unlikely, based on information available.

Bioaccumulative Potential Bioaccumulation is unlikely

Mobility in soil The product is water soluble, and may spread in water systems Will likely be mobile in the environment due to its water solubility Highly mobile in soils

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors
Persistent Organic Pollutant This product does not contain any known or suspected substance
Ozone Depletion Potential This product does not contain any known or suspected substance

SECTION 13. DISPOSAL CONSIDERATIONS

Waste from Residues/Unused Products Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

Contaminated Packaging Dispose of this container to hazardous or special waste collection point.

Other Information Waste codes should be assigned by the user based on the application for which the product was used. Do not empty into drains.

SECTION 14. TRANSPORT INFORMATION

Road and Rail Transport

UN-No	UN3276
Proper Shipping Name	NITRILES, LIQUID, TOXIC, N.O.S.
Hazard Class	6.1
Packing Group	III

IMDG/IMO

UN-No	UN3276
Proper Shipping Name	NITRILES, LIQUID, TOXIC, N.O.S.
Hazard Class	6.1
Packing Group	III

SAFETY DATA SHEET

3,5-Bis(trifluoromethyl)benzotrile

IATA

UN-No UN3276
Proper Shipping Name NITRILES, LIQUID, TOXIC, N.O.S.
Hazard Class 6.1
Packing Group III

Special Precautions for User No special precautions required

SECTION 15. REGULATORY INFORMATION
International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

Component	The Inventory of Hazardous Chemicals (2015 Edition)	List of dangerous goods GB 12268 - 2012	TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
3,5-Bis(trifluoromethyl)benzotrile	-	-	X	-	248-240-7	-	-	-	-		-	-

National Regulations
SECTION 16. OTHER INFORMATION

Prepared By Health, Safety and Environmental Department
Revision Date 27-Apr-2024
Revision Summary New emergency telephone response service provider.

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.

First aid for chemical exposure, including the use of eye wash and safety showers.

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer

PNEC - Predicted No Effect Concentration

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

3,5-Bis(trifluoromethyl)benzotrile

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

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 Safety Data Sheet