

ALFAAA19576

## 3,5-Bis(trifluoromethyl)phenylacetonitrile

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

产品说明:  
Product Description: 3,5-二(三氟甲基)苯乙腈,  
3,5-Bis(trifluoromethyl)phenylacetonitrile

Cat No. : A19576  
CAS No 85068-32-2  
Molecular Formula C10H5F6N

Supplier Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

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

E-mail address begel.sdsdesk@thermofisher.com

Recommended Use Laboratory chemicals.  
Uses advised against No Information available

### SECTION 2. HAZARD IDENTIFICATION

Physical State  
Liquid

Appearance  
Yellow

Odor  
No information available

#### Emergency Overview

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

#### Classification of the substance or mixture

Acute Oral Toxicity	Category 4
Acute Dermal Toxicity	Category 4
Acute Inhalation Toxicity - Vapors	Category 4

#### Label Elements



Signal Word

Warning

Hazard Statements

# SAFETY DATA SHEET

## 3,5-Bis(trifluoromethyl)phenylacetonitrile

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

### Precautionary Statements

#### Prevention

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

#### Response

P302 + P352 - IF ON SKIN: Wash with plenty of soap and water  
P304 + P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing  
P312 - Call a POISON CENTER or doctor if you feel unwell  
P330 - Rinse mouth  
P362 + P364 - Take off contaminated clothing and wash it before reuse

#### Storage

P403 - Store in a well-ventilated place

#### Disposal

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

### Physical and Chemical Hazards

None identified.

### 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. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil. The product is insoluble and sinks in water.

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)phenyl]acetonitrile	85068-32-2	98

## SECTION 4. FIRST AID MEASURES

### General Advice

If symptoms persist, call a physician.

### 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 plenty of water for at least 15 minutes. If skin irritation persists, call a physician.

### Inhalation

Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.

### Ingestion

Clean mouth with water and drink afterwards plenty of water.

### Most important symptoms and effects

None reasonably foreseeable.

### 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**

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Thermal decomposition can lead to release of irritating gases and vapors.

**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**

Ensure adequate ventilation. Use personal protective equipment as required.

**Environmental Precautions**

Should not be released into the environment.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation.

**Storage**

Keep container tightly closed in a dry and well-ventilated place.

**Specific Use(s)**

Use in laboratories

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

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### Personal protective equipment

**Eye Protection** Wear safety glasses with side shields (or goggles) (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Nitrile rubber	See manufacturers	-	EN 374	(minimum requirement)
Neoprene	recommendations			
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** Long sleeved clothing

**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

<b>Appearance</b>	Yellow	
<b>Physical State</b>	Liquid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>		
<b>Melting Point/Range</b>	No data available	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	No information available	
<b>Flash Point</b>	> 110 °C / > 230 °F	<b>Method -</b> No information available
<b>Evaporation Rate</b>	No data available	
<b>Flammability (solid,gas)</b>	Not applicable	Liquid
<b>Explosion Limits</b>	No data available	
<b>Vapor Pressure</b>	No data available	
<b>Vapor Density</b>	No data available	(Air = 1.0)
<b>Specific Gravity / Density</b>	1.4200	
<b>Bulk Density</b>	Not applicable	Liquid

# SAFETY DATA SHEET

## 3,5-Bis(trifluoromethyl)phenylacetonitrile

Water Solubility	Immiscible
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	No information available
Oxidizing Properties	No information available
Molecular Formula	C10H5F6N
Molecular Weight	253.15

### SECTION 10. STABILITY AND REACTIVITY

Stability	Stable under normal conditions.
Hazardous Reactions	None under normal processing.
Hazardous Polymerization	No information available.
Conditions to Avoid	None known.
Materials to avoid	Oxidizing agent.

**Hazardous Decomposition Products** Carbon monoxide (CO). Nitrogen oxides (NOx). Hydrogen fluoride. Hydrogen cyanide (hydrocyanic acid).

### 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.

# SAFETY DATA SHEET

## 3,5-Bis(trifluoromethyl)phenylacetonitrile

(j) aspiration hazard; No data available

Symptoms / effects, both acute and delayed No information available

### 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** Immiscible with water.

**Bioaccumulative Potential** May have some potential to bioaccumulate

**Mobility in soil** Spillage unlikely to penetrate soil The product is insoluble and sinks in water Is not likely mobile in the environment due its low water solubility

**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.  
**Technical Shipping Name** 3,5-Bis(trifluoromethyl)phenylacetonitrile  
**Hazard Class** 6.1  
**Packing Group** III

#### IMDG/IMO

**UN-No** UN3276  
**Proper Shipping Name** NITRILES, LIQUID, TOXIC, N.O.S.  
**Technical Shipping Name** 3,5-Bis(trifluoromethyl)phenylacetonitrile  
**Hazard Class** 6.1  
**Packing Group** III

#### IATA

# SAFETY DATA SHEET

## 3,5-Bis(trifluoromethyl)phenylacetoneitrile

**UN-No** UN3276  
**Proper Shipping Name** NITRILES, LIQUID, TOXIC, N.O.S.  
**Technical Shipping Name** 3,5-Bis(trifluoromethyl)phenylacetoneitrile  
**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)phenyl]acetoneitrile	-	-	X	-	285-294-0	-	-	-	-		-	-

#### National Regulations

### SECTION 16. OTHER INFORMATION

**Prepared By** Health, Safety and Environmental Department  
**Revision Date** 25-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

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## 3,5-Bis(trifluoromethyl)phenylacetonitrile

**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**