

ALFAAA14951

## 2-(Trifluoromethyl)benzonitrile

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

产品说明:  
Product Description: 2-(三氟甲基)苯甲腈  
2-(Trifluoromethyl)benzonitrile

Cat No. : A14951  
Synonyms 2-(Trifluoromethyl)benzonitrile  
CAS No 447-60-9  
Molecular Formula C8H4F3N

Supplier Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
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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**  
Light yellow

**Odor**  
No information available

#### Emergency Overview

Combustible liquid. Toxic if swallowed. Toxic in contact with skin. Causes skin irritation. Causes serious eye irritation. Toxic if inhaled. May cause respiratory irritation.

#### Classification of the substance or mixture

Flammable liquids.	Category 4
Acute Oral Toxicity	Category 3
Acute Dermal Toxicity	Category 3
Acute Inhalation Toxicity - Vapors	Category 3
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 2
Specific target organ toxicity - (single exposure)	Category 3

#### Label Elements

# SAFETY DATA SHEET

## 2-(Trifluoromethyl)benzonitrile

**Signal Word****Danger****Hazard Statements**

H227 - Combustible liquid  
H315 - Causes skin irritation  
H319 - Causes serious eye irritation  
H335 - May cause respiratory irritation  
H301 + H311 + H331 - Toxic if swallowed, in contact with skin or if inhaled

**Precautionary Statements****Prevention**

P261 - Avoid breathing dust/fume/gas/mist/vapors/spray  
P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking  
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**

P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P301 + P310 - IF SWALLOWED: Immediately call a POISON CENTER or doctor  
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  
P311 - Call a POISON CENTER or doctor  
P330 - Rinse mouth  
P370 + P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish  
P361 + P364 - Take off immediately all contaminated clothing and wash it before reuse

**Storage**

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed  
P405 - Store locked up

**Disposal**

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

**Physical and Chemical Hazards**

Combustible material.

**Health Hazards**

Toxic if swallowed. Toxic in contact with skin. Causes skin irritation. Causes serious eye irritation. Toxic if inhaled. May cause respiratory irritation.

**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. The product evaporates slowly.

**Other Hazards**

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

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Component	CAS No	Weight %
.alpha.,.alpha.,.alpha.-Trifluoro-2-toluonitrile	447-60-9	>=90

**SECTION 4. FIRST AID MEASURES****General Advice**

Show this safety data sheet to the doctor in attendance. Immediate medical attention is required.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. In the case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

**Skin Contact**

Wash off immediately with plenty of water for at least 15 minutes. Immediate medical attention is required.

**Inhalation**

Remove to fresh air. If not breathing, give artificial respiration. Do not use mouth-to-mouth method if victim ingested or inhaled the substance; give artificial respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Immediate medical attention is required.

**Ingestion**

Do NOT induce vomiting. Call a physician or poison control center immediately.

**Most important symptoms and effects**

. 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 (CO<sub>2</sub>), dry chemical, alcohol-resistant 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. Thermal decomposition can lead to release of irritating gases and vapors.

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

Ensure adequate ventilation. Use personal protective equipment as required. Keep people away from and upwind of spill/leak. Evacuate personnel to safe areas. Remove all sources of ignition. Take precautionary measures against static discharges.

**Environmental Precautions**

Should not be released into the environment. Do not flush into surface water or sanitary sewer system.

**Methods for Containment and Clean Up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition.

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Refer to protective measures listed in Sections 8 and 13.

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

Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Use only under a chemical fume hood. Do not breathe mist/vapors/spray. Do not ingest. If swallowed then seek immediate medical assistance. Keep away from open flames, hot surfaces and sources of ignition.

**Storage**

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

**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 that eyewash stations and safety showers are close to the workstation location. 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	-	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

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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**

Prevent product from entering drains.

**SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

<b>Appearance</b>	Light yellow	
<b>Physical State</b>	Liquid	
<b>Odor</b>	No information available	
<b>Odor Threshold</b>	No data available	
<b>pH</b>	No information available	
<b>Melting Point/Range</b>	7.5 °C / 45.5 °F	
<b>Softening Point</b>	No data available	
<b>Boiling Point/Range</b>	204 - 206 °C / 399.2 - 402.8 °F	@ 760 mmHg
<b>Flash Point</b>	90 °C / 194 °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>	5.90	(Air = 1.0)
<b>Specific Gravity / Density</b>	1.2940	
<b>Bulk Density</b>	Not applicable	Liquid
<b>Water Solubility</b>	Insoluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>Viscosity</b>	No data available	
<b>Explosive Properties</b>		explosive air/vapour mixtures possible
<b>Oxidizing Properties</b>	No information available	
<b>Molecular Formula</b>	C8H4F3N	
<b>Molecular Weight</b>	171.12	
<b>Refractive index</b>	1.4622-1.4642	

**SECTION 10. STABILITY AND REACTIVITY**

<b>Stability</b>	Stable under normal conditions.
<b>Hazardous Reactions</b>	None under normal processing.
<b>Hazardous Polymerization</b>	No information available.
<b>Conditions to Avoid</b>	Incompatible products. Keep away from open flames, hot surfaces and sources of ignition.
<b>Materials to avoid</b>	Strong oxidizing agents.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrogen oxides (NO<sub>x</sub>). Hydrogen fluoride.

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

(a) acute toxicity;

(b) skin corrosion/irritation; Category 2

(c) serious eye damage/irritation; Category 2

(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; Category 3

Results / Target organs Respiratory system

(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 a substance which is: Harmful to aquatic organisms. The product contains following substances which are hazardous for the environment.

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
.alpha.,.alpha.,.alpha.-Trifluoro-2-toluenitrile	LC50: 38.5 - 46.4 mg/L, 96h flow-through (Pimephales promelas)			

## Persistence and Degradability

## Persistence

Insoluble in water, May persist, based on information available.

## Degradation in sewage treatment plant

Contains substances known to be hazardous to the environment or not degradable in waste water treatment plants.

## Bioaccumulative Potential

May have some potential to bioaccumulate

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

**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** Do not flush to sewer. 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** .alpha.,.alpha.,.alpha.-Trifluoro-2-toluenitrile  
**Hazard Class** 6.1  
**Packing Group** III

IMDG/IMO

**UN-No** UN3276  
**Proper Shipping Name** NITRILES, LIQUID, TOXIC, N.O.S.  
**Technical Shipping Name** .alpha.,.alpha.,.alpha.-Trifluoro-2-toluenitrile  
**Hazard Class** 6.1  
**Packing Group** III

IATA

**UN-No** UN3276  
**Proper Shipping Name** NITRILES, LIQUID, TOXIC, N.O.S.  
**Technical Shipping Name** .alpha.,.alpha.,.alpha.-Trifluoro-2-toluenitrile  
**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

## 2-(Trifluoromethyl)benzonitrile

.alpha.,.alpha.,.alpha.- Trifluoro-2-toluenitrile	-	-	X	-	207-184-3	-	-	-	-	-	-
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## 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/NDL** - 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

**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**