

ALFAAA14514

4-(Trifluoromethyl)benzotrile

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

产品说明:
Product Description: 4-(三氟甲基)苯甲腈
4-(Trifluoromethyl)benzotrile

Cat No. : A14514
CAS No 455-18-5
Molecular Formula C8 H4 F3 N

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
Solid

Appearance
White

Odor
pungent

Emergency Overview

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

Classification of the substance or mixture

| | |
|--|------------|
| Acute Oral Toxicity | Category 4 |
| Acute Dermal Toxicity | Category 4 |
| Acute Inhalation Toxicity - Dusts and Mists | Category 4 |
| Skin Corrosion/Irritation | Category 2 |
| Serious Eye Damage/Eye Irritation | Category 2 |
| Specific target organ toxicity - (single exposure) | Category 3 |

Label Elements



Signal Word**Warning****Hazard Statements**

H315 - Causes skin irritation
H319 - Causes serious eye irritation
H335 - May cause respiratory irritation
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

P330 - Rinse mouth
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
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P312 - Call a POISON CENTER or doctor if you feel unwell
P362 + P364 - Take off contaminated clothing and wash it before reuse

Storage

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

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. Causes skin irritation. Causes serious eye irritation. Harmful 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.

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

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

| Component | CAS No | Weight % |
|------------------------------------|----------|----------|
| Benzonitrile, 4-(trifluoromethyl)- | 455-18-5 | >95 |

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

If symptoms persist, call a physician. Show this safety data sheet to the doctor in attendance. Do not breathe dust/fume/gas/mist/vapors/spray. Do not get in eyes, on skin, or on clothing.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Immediate medical attention is required.

Skin Contact

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

Inhalation

Remove to fresh air. 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. If not breathing, give artificial respiration.

Ingestion

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

Most important symptoms and effects

No information available.

Self-Protection of the First Aider

Use personal protective equipment as required.

Notes to Physician

Treat symptomatically.

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

Water spray, carbon dioxide (CO₂), 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. Avoid dust formation. Remove all sources of ignition. Take precautionary measures against static discharges.

Environmental Precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

Methods for Containment and Clean Up

Sweep up and shovel into suitable containers for disposal. Avoid dust formation. Remove all sources of ignition.

Refer to protective measures listed in Sections 8 and 13.

SECTION 7. HANDLING AND STORAGE**Handling**

Use only under a chemical fume hood. Wear personal protective equipment/face protection. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. 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

4-(Trifluoromethyl)benzonitrile

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. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust MDHS70 General methods for sampling airborne gases and vapours

Exposure Controls

Engineering Measures

Use only under a chemical fume hood. 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 Wear safety glasses with side shields (or goggles) 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 No protective equipment is needed under normal use conditions.

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

Small scale/Laboratory use Maintain adequate ventilation

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

Environmental exposure controls Do not allow material to contaminate ground water system.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance White
Physical State Solid

Odor pungent
Odor Threshold No data available
pH No information available

4-(Trifluoromethyl)benzonitrile

| | | |
|--|--------------------------------------|--|
| Melting Point/Range | 37 - 38 °C / 98.6 - 100.4 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | No information available - 185 - 365 | |
| Flash Point | 71 °C / 159.8 °F | Method - No information available |
| Evaporation Rate | Not applicable | Solid |
| Flammability (solid,gas) | No information available | |
| Explosion Limits | No data available | |
| Vapor Pressure | No data available | |
| Vapor Density | Not applicable | Solid |
| Specific Gravity / Density | 1.270 | |
| Bulk Density | No data available | |
| Water Solubility | Insoluble | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Component | log Pow | |
| Benzonitrile, 4-(trifluoromethyl)- | 2.5 | |
| Autoignition Temperature | No data available | |
| Decomposition Temperature | > 280°C | |
| Viscosity | Not applicable | Solid |
| Explosive Properties | | explosive air/vapour mixtures possible |
| Oxidizing Properties | No information available | |
| Molecular Formula | C8 H4 F3 N | |
| Molecular Weight | 171.12 | |

SECTION 10. STABILITY AND REACTIVITY

| | |
|---|---|
| Stability | Stable under normal conditions. |
| Hazardous Reactions | None under normal processing. |
| Hazardous Polymerization | No information available. |
| Conditions to Avoid | Incompatible products. Excess heat. Avoid dust formation. Keep away from open flames, hot surfaces and sources of ignition. |
| Materials to avoid | Strong oxidizing agents. Reducing Agent. |
| Hazardous Decomposition Products | Carbon monoxide (CO). Carbon dioxide (CO ₂). Nitrogen oxides (NO _x). 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 |

SAFETY DATA SHEET

4-(Trifluoromethyl)benzonitrile

| | |
|--|--|
| (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; | Not applicable Solid |
| Other Adverse Effects | The toxicological properties have not been fully investigated. |
| Symptoms / effects,both acute and delayed | No information available |

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects Do not empty into drains. .

Persistence and Degradability
Persistence Persistence is unlikely.

Bioaccumulative Potential Bioaccumulation is unlikely

| Component | log Pow | Bioconcentration factor (BCF) |
|------------------------------------|---------|-------------------------------|
| Benzonitrile, 4-(trifluoromethyl)- | 2.5 | No data available |

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

4-(Trifluoromethyl)benzotrile**Road and Rail Transport**

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class 6.1
Packing Group III

IMDG/IMO

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, TOXIC, N.O.S.
Hazard Class 6.1
Packing Group III

IATA

UN-No UN3439
Proper Shipping Name NITRILES, SOLID, 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/NDL), 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 |
|----------------------------------|---|---|------|-------|-----------|------|-----|-------|------|------|------|------|
| Benzotrile, 4-(trifluoromethyl)- | - | - | X | X | 207-239-1 | X | - | X | - | X | - | - |

National Regulations**SECTION 16. OTHER INFORMATION**

Prepared By Health, Safety and Environmental Department
Revision Date 22-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

4-(Trifluoromethyl)benzonitrile

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

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

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

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