

ALFAAA17029

3-(Trifluoromethyl)benzonitrile

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

产品说明:
Product Description: 3-(三氟甲基)苯甲腈, 98%
3-(Trifluoromethyl)benzonitrile

Cat No. : A17029
Synonyms 3-(Trifluoromethyl)benzonitrile
CAS No 368-77-4
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
Liquid

Appearance
Yellow-orange

Odor
Fishy

Emergency Overview

Combustible liquid. 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

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

3-(Trifluoromethyl)benzonitrile

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

H227 - Combustible liquid
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**

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
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
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
P330 - Rinse mouth
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 + 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

Combustible material.

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.

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-m-toluonitrile | 368-77-4 | >95 |

SECTION 4. FIRST AID MEASURES**Eye Contact**

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

Skin Contact

3-(Trifluoromethyl)benzonitrile

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

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, 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**

Use personal protective equipment as required. 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. 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. Use spark-proof tools and explosion-proof equipment.

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. Use only non-sparking tools. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges.

3-(Trifluoromethyl)benzonitrile

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**

Use only under a chemical fume hood. Ensure that eyewash stations and safety showers are close to the workstation location. Use explosion-proof electrical/ventilating/lighting equipment. 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 | - | 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 compatability, 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

3-(Trifluoromethyl)benzonitrile

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

| | | |
|---|--------------------------|--|
| Appearance | Yellow-orange | |
| Physical State | Liquid | |
| Odor | Fishy | |
| Odor Threshold | No data available | |
| pH | No information available | |
| Melting Point/Range | 14.5 °C / 58.1 °F | |
| Softening Point | No data available | |
| Boiling Point/Range | 189 °C / 372.2 °F | @ 760 mmHg |
| 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 | |
| Vapor Pressure | No data available | |
| Vapor Density | 5.90 | (Air = 1.0) |
| Specific Gravity / Density | 1.280 | |
| Bulk Density | Not applicable | Liquid |
| Water Solubility | No information available | |
| Solubility in other solvents | No information available | |
| Partition Coefficient (n-octanol/water) | | |
| Component | log Pow | |
| .alpha.,.alpha.,.alpha.-Trifluoro-m-toluo nitrile | 2.5 | |
| 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 | 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. 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 (CO₂). 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

(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

Other Adverse Effects

The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity effects

Do not empty into drains. 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-m-toluenitrile | LC50: 39.3 - 57.9 mg/L, 96h flow-through (Pimephales promelas) | | | |

Persistence and Degradability

Persistence

No information available

Degradation in sewage

Persistence is unlikely.

treatment plant

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

Bioaccumulative Potential

Bioaccumulation is unlikely

| Component | log Pow | Bioconcentration factor (BCF) |
|--|---------|-------------------------------|
| .alpha.,.alpha.,.alpha.-Trifluoro-m-toluenitrile | 2.5 | No data available |

Mobility in soil No information available

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.
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

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/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 |
|--|---|---|------|-------|-----------|------|-----|-------|------|------|------|------|
| .alpha.,.alpha.,.alpha.-Trifluoro-m-toluonitrile | - | - | X | X | 206-711-4 | - | - | X | - | | - | - |

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