

## Chemical Safety Data Sheet MSDS / SDS

**2-(TRIFLUOROMETHOXY)BENZONITRILE**

Revision Date:2026-05-31 Revision Number:1

**SECTION 1: Identification of the substance/mixture and of the company/undertaking****Product identifier**

Product name : 2-(TRIFLUOROMETHOXY)BENZONITRILE  
CBnumber : CB8686824  
CAS : 63968-85-4  
EINECS Number : 264-584-0  
Synonyms : 2-(Trifluoromethoxy)benzotrile

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.  
Uses advised against : none

**Company Identification**

Company : Chemicalbook  
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing  
Telephone : 010-86108875

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

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

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position 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.

Continuerinsing.

P405 Store locked up.

**Hazard statements**

H302 Harmful if swallowed

H312 Harmful in contact with skin

H315 Causes skin irritation

H319 Causes serious eye irritation

H331 Toxic if inhaled

H335 May cause respiratory irritation

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 2-(TRIFLUOROMETHOXY)BENZONITRILE
Synonyms	: 2-(Trifluoromethoxy)benzotrile
CAS	: 63968-85-4
EC number	: 264-584-0
MF	: C8H4F3NO
MW	: 187.12

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## 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.

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## SECTION 5: Firefighting 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.

## NFPA 704



HEALTH 2 Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

SPEC.

HAZ.

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## 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. See Section 12 for additional Ecological Information.

### 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

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## 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 MDHS 88

Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

#### Exposure Controls

#### Engineering Measures

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

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.

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## SECTION 9: Physical and chemical properties

### **Information on basic physicochemical properties**

No information available

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#### **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**

80 - 82 °C / 176 - 179.6 °F

### **Flash Point**

No information available

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**

No data available (Air = 1.0)

### **Specific Gravity / Density**

1,245 g/cm<sup>3</sup>

### **Bulk Density**

Not applicable Liquid

### **Water Solubility**

No information available

### **Solubility in other solvents**

No information available

### **Partition Coefficient (n-octanol/water)**

No data available

### **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**

C<sub>8</sub> H<sub>4</sub> F<sub>3</sub> N O

**Molecular Weight**

187.12

**Colour**

Colorless to Yellow

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**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**

No information available.

**Hazardous Decomposition Products**

None under normal use conditions.

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**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**

No information available

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## 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**

No information available

### **Persistence**

Persistence is unlikely, based on information available.

### **Bioaccumulative Potential**

Bioaccumulation is unlikely

### **Mobility in soil**

The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces Will likely be mobile in the environment due to its volatility Disperses rapidly in air

### **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

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## 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.

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## SECTION 14: Transport information

### **Road and Rail Transport**

#### **UN-No**

UN3276

#### **Proper Shipping Name**

NITRILES, LIQUID, TOXIC, N.O.

#### **Technical Shipping Name**

(2-(Trifluoromethoxy)benzotrile)

#### **Hazard Class**

6.1

**Packing Group**

III

**IMDG/IMO**

**UN-No**

UN3276

**Proper Shipping Name**

NITRILES, LIQUID, TOXIC, N.O.

**Technical Shipping Name**

(2-(Trifluoromethoxy)benzotrile)

**Hazard Class**

6.1

**Packing Group**

III

**IATA**

**UN-No**

UN3276

**Proper Shipping Name**

NITRILES, LIQUID, TOXIC, N.O.

**Technical Shipping Name**

(2-(Trifluoromethoxy)benzotrile)

**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	TCS	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
2-(Trifluoromethoxy)benzotrile	-	-	X	-	264-584-0	-	-	-	-	-	-	-

### SECTION 16: Other information

#### Prepared By

Health, Safety and Environmental Department

#### Revision Date

23-Sep-2025

#### Revision Summary

Not applicable.

#### 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

##### TSCA

United States Toxic Substances Control Act Section 8(b)

Inventory

##### EINECS/ELINCS

European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

##### DSL/NDSL

Canadian Domestic Substances List/Non-Domestic Substances List

##### PICCS

Philippines Inventory of Chemicals and Chemical Substances

##### ENCS

Japanese Existing and New Chemical Substances

##### IECSC

Chinese Inventory of Existing Chemical Substances

##### AICS

Australian Inventory of Chemical Substances

##### KECL

Korean Existing and Evaluated Chemical Substances

##### NZIoC

New Zealand Inventory of Chemicals

**WEL**

Workplace Exposure Limit

**TWA**

Time Weighted Average

**ACGIH**

American Conference of Governmental Industrial Hygienists

**IARC**

International Agency for Research on Cancer

**DNEL**

Derived No Effect Level

**PNEC**

Predicted No Effect Concentration

**RPE**

Respiratory Protective Equipment

**LD50**

Lethal Dose 50%

**LC50**

Lethal Concentration 50%

**EC50**

Effective Concentration 50%

**NOEC**

No Observed Effect Concentration

**POW**

Partition coefficient Octanol:Water

**PBT**

Persistent, Bioaccumulative, Toxic

**vPvB**

very Persistent, very Bioaccumulative

**ICAO/IATA**

International Civil Aviation Organization/International Air

Transport Association

**IMO/IMDG**

International Maritime Organization/International Maritime

Dangerous Goods Code

**ADR**

European Agreement Concerning the International Carriage of

Dangerous Goods by Road

**MARPOL**

International Convention for the Prevention of Pollution from

Ships

**OECD**

Organisation for Economic Co-operation and Development

**ATE**

Acute Toxicity Estimate

**BCF**

Bioconcentration factor

**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

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