

# 4-(Trifluoromethyl)benzonitrile

## Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations  
SDS ID: 3837304  
Issue date: 4/30/2025 Version: 1.0

### SECTION 1: Identification

#### 1.1. Identification

Product form : Substance  
Substance name : 4-(Trifluoromethyl)benzonitrile  
CAS-No. : 455-18-5  
Product code : 3837-3-04  
Formula : C<sub>8</sub>H<sub>4</sub>F<sub>3</sub>N  
Synonyms : PTF-CN  
Other means of identification : MFCD00001826

#### 1.2. Recommended use and restrictions on use

Use of the substance/mixture : Laboratory chemicals  
Manufacture of substances  
Scientific research and development

#### 1.3. Supplier

SynQuest Laboratories, Inc.  
P.O. Box 309  
Alachua, FL, Alachua, 32615  
United States of America  
T (386) 462-0788 - F (386) 462-7097  
[info@synquestlabs.com](mailto:info@synquestlabs.com) - [www.synquestlabs.com](http://www.synquestlabs.com)

#### 1.4. Emergency telephone number

Emergency number : (844) 523-4086 (3E Company - Account 10069)

### SECTION 2: Hazard(s) identification

#### 2.1. Classification of the substance or mixture

##### GHS US classification

Acute toxicity (oral) Category 3	H301	Toxic if swallowed
Acute toxicity (dermal) Category 3	H311	Toxic in contact with skin
Acute toxicity (inhalation) Category 4	H332	Harmful if inhaled
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Specific target organ toxicity – Single exposure, Category 3, Respiratory tract irritation	H335	May cause respiratory irritation

Full text of H statements : see section 16

#### 2.2. GHS Label elements, including precautionary statements

##### GHS US labeling

Hazard pictograms (GHS US) :



Signal word (GHS US) :

Danger

Hazard statements (GHS US) :

H301+H311 - Toxic if swallowed or in contact with skin  
H315 - Causes skin irritation

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Precautionary statements (GHS US)	H319 - Causes serious eye irritation
	H332 - Harmful if inhaled
	H335 - May cause respiratory irritation
	P261 - Avoid breathing fumes, mist, spray, vapors.
	P264 - Wash 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.
	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.
	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/physician if you feel unwell
	P321 - Specific treatment (see supplemental first aid instructions on this label)
	P322 - Specific treatment (see supplemental first aid instruction on this label)
	P330 - Rinse mouth.
	P332+P313 - If skin irritation occurs: Get medical advice/attention.
	P337+P313 - If eye irritation persists: Get medical advice/attention.
	P361+P364 - Take off immediately all contaminated clothing and wash it before reuse.
	P362+P364 - Take off contaminated clothing and wash it before reuse.
	P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
	P405 - Store locked up.
	P501 - Dispose of contents/container to an approved waste disposal plant

### 2.3. Other hazards which do not result in classification

No additional information available

### 2.4. Unknown acute toxicity (GHS US)

No additional information available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Substance type : Mono-constituent

Name	Product identifier	%	GHS US classification
4-(Trifluoromethyl)benzonitrile (Main constituent)	CAS-No.: 455-18-5	≤ 100	Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Acute Tox. 4 (Inhalation), H332 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

Full text of hazard classes and H-statements : see section 16

### 3.2. Mixtures

Not applicable

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### SECTION 4: First-aid measures

#### 4.1. Description of first aid measures

First-aid measures general	: In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). Move the affected personnel away from the contaminated area.
First-aid measures after inhalation	: Remove person to fresh air and keep comfortable for breathing. If not breathing, give artificial respiration. Get immediate medical advice/attention.
First-aid measures after skin contact	: Wash with plenty of soap and water. Get immediate medical advice/attention.
First-aid measures after eye contact	: Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Get immediate medical advice/attention.
First-aid measures after ingestion	: Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth out with water. Get immediate medical advice/attention.

#### 4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.
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#### 4.3. Immediate medical attention and special treatment, if necessary

Treat symptomatically.

### SECTION 5: Fire-fighting measures

#### 5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	: Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.
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#### 5.2. Specific hazards arising from the chemical

Fire hazard	: Thermal decomposition generates: Carbon oxides. Hydrogen fluoride. Nitrogen oxides.
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#### 5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: In case of fire: Evacuate area.
Protection during firefighting	: Wear gas tight chemically protective clothing in combination with self contained breathing apparatus. For further information refer to section 8: "Exposure controls/personal protection".

### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

General measures	: Evacuate unnecessary personnel. Ensure adequate air ventilation. Do not breathe dust.
<b>6.1.1. For non-emergency personnel</b>	
Emergency procedures	: Only qualified personnel equipped with suitable protective equipment may intervene.
<b>6.1.2. For emergency responders</b>	
Protective equipment	: Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".

#### 6.2. Environmental precautions

Avoid release to the environment. Notify authorities if product enters sewers or public waters.

#### 6.3. Methods and material for containment and cleaning up

For containment	: Stop leak if safe to do so.
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Methods for cleaning up	: Sweep or shovel spills into appropriate container for disposal. Minimize generation of dust.
Other information	: For disposal of solid materials or residues refer to section 13 : "Disposal considerations".

### 6.4. Reference to other sections

No additional information available

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

Precautions for safe handling	: Do not handle until all safety precautions have been read and understood. Ensure good ventilation of the work station. Do not breathe dust, mist, spray. Wear personal protective equipment. Avoid contact with skin and eyes.
Hygiene measures	: Handle in accordance with good industrial hygiene and safety procedures. Do not eat, drink or smoke when using this product. Always wash hands after handling the product.

### 7.2. Conditions for safe storage, including any incompatibilities

Technical measures	: Comply with applicable regulations.
Storage conditions	: Keep container closed when not in use.
Incompatible materials	: Refer to Section 10 on Incompatible Materials.
Storage area	: Store in dry, cool, well-ventilated area.

## SECTION 8: Exposure controls/personal protection

### 8.1. Control parameters

No additional information available

### 8.2. Appropriate engineering controls

No additional information available

### 8.3. Individual protection measures/Personal protective equipment

No additional information available

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Low melting solid.
Color	: No data available
Odor	: No data available
Odor threshold	: No data available
pH	: No data available
Melting point	: 39 – 41 °C
Freezing point	: No data available
Boiling point	: 80 – 81 °C (@ 20 mm Hg)
Flash point	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Flammability (solid, gas)	: No data available
Vapor pressure	: No data available
Relative vapor density at 20 °C	: No data available
Relative density	: No data available
Density	: 1.278 g/ml (@ 25 °C)

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Molecular mass	: 171.122 g/mol
Solubility	: No data available
Partition coefficient n-octanol/water (Log Pow)	: No data available
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available
Explosion limits	: No data available
Explosive properties	: No data available
Oxidizing properties	: No data available

### 9.2. Other information

Refractive index	: 1.4583 (@ 20 °C)
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## SECTION 10: Stability and reactivity

### 10.1. Reactivity

No additional information available

### 10.2. Chemical stability

The product is stable at normal handling and storage conditions.

### 10.3. Possibility of hazardous reactions

No additional information available

### 10.4. Conditions to avoid

Keep away from heat, sparks and flame.

### 10.5. Incompatible materials

Oxidizing agents. Reducing agents. Strong acids.

### 10.6. Hazardous decomposition products

Under normal conditions of storage and use, hazardous decomposition products should not be produced. Hazardous decomposition products in case of fire, see Section 5.

## SECTION 11: Toxicological information

### 11.1. Information on toxicological effects

Acute toxicity (oral)	: Toxic if swallowed.
Acute toxicity (dermal)	: Toxic in contact with skin.
Acute toxicity (inhalation)	: Harmful if inhaled.

4-(Trifluoromethyl)benzonitrile (455-18-5)	
ATE US (oral)	100 mg/kg body weight
ATE US (dermal)	300 mg/kg body weight
ATE US (gases)	4500 ppmV/4h
ATE US (vapors)	11 mg/l/4h
ATE US (dust, mist)	1.5 mg/l/4h
Skin corrosion/irritation	: Causes skin irritation.

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Serious eye damage/irritation	: Causes serious eye irritation.
Respiratory or skin sensitization	: Not classified
Germ cell mutagenicity	: Not classified
Carcinogenicity	: Not classified
Reproductive toxicity	: Not classified
STOT-single exposure	: May cause respiratory irritation.
STOT-repeated exposure	: Not classified
Aspiration hazard	: Not classified
Viscosity, kinematic	: No data available
Symptoms/effects	: The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11.

## SECTION 12: Ecological information

### 12.1. Toxicity

No additional information available

### 12.2. Persistence and degradability

#### 4-(Trifluoromethyl)benzonitrile (455-18-5)

Persistence and degradability	Rapidly degradable
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### 12.3. Bioaccumulative potential

No additional information available

### 12.4. Mobility in soil

No additional information available

### 12.5. Other adverse effects

No additional information available

## SECTION 13: Disposal considerations

### 13.1. Disposal methods

Waste treatment methods	: Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber.
Product/Packaging disposal recommendations	: Dispose of contents/container in accordance with licensed collector's sorting instructions.
Additional information	: Recycle the material as far as possible.

## SECTION 14: Transport information

### 14.1. UN number

DOT NA No	: UN3439
UN-No. (TDG)	: UN3439
UN-No. (IMDG)	: 3439
UN-No. (IATA)	: 3439

### 14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Nitriles, solid, toxic, n.o.s.
Proper Shipping Name (TDG)	: NITRILES, SOLID, TOXIC, N.O.S.
Proper Shipping Name (IMDG)	: NITRILES, SOLID, TOXIC, N.O.S.

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Proper Shipping Name (IATA) : Nitriles, solid, toxic, n.o.s.

### 14.3. Transport hazard class(es)

#### DOT

Transport hazard class(es) (DOT) : 6.1

Hazard labels (DOT) : 6.1



#### TDG

Transport hazard class(es) (TDG) : 6.1

Hazard labels (TDG) : 6.1



#### IMDG

Transport hazard class(es) (IMDG) : 6.1

Hazard labels (IMDG) : 6.1



#### IATA

Transport hazard class(es) (IATA) : 6.1

Hazard labels (IATA) : 6.1



### 14.4. Packing group

Packing group (DOT) : III

Packing group (TDG) : III

Packing group (IMDG) : III

Packing group (IATA) : III

### 14.5. Environmental hazards

Other information : No supplementary information available.

### 14.6. Special precautions for user

#### DOT

UN-No.(DOT) : UN3439

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DOT Special Provisions (49 CFR 172.102)	: IB8 - Authorized IBCs: Metal (11A, 11B, 11N, 21A, 21B, 21N, 31A, 31B and 31N); Rigid plastics (11H1, 11H2, 21H1, 21H2, 31H1 and 31H2); Composite (11HZ1, 11HZ2, 21HZ1, 21HZ2, 31HZ1 and 31HZ2); Fiberboard (11G); Wooden (11C, 11D and 11F); Flexible (13H1, 13H2, 13H3, 13H4, 13H5, 13L1, 13L2, 13L3, 13L4, 13M1 or 13M2). IP3 - Flexible IBCs must be sift-proof and water-resistant or must be fitted with a sift-proof and water-resistant liner. T1 - 1.5 178.274(d)(2) Normal..... 178.275(d)(2) TP33 - The portable tank instruction assigned for this substance applies for granular and powdered solids and for solids which are filled and discharged at temperatures above their melting point which are cooled and transported as a solid mass. Solid substances transported or offered for transport above their melting point are authorized for transportation in portable tanks conforming to the provisions of portable tank instruction T4 for solid substances of packing group III or T7 for solid substances of packing group II, unless a tank with more stringent requirements for minimum shell thickness, maximum allowable working pressure, pressure-relief devices or bottom outlets are assigned in which case the more stringent tank instruction and special provisions shall apply. Filling limits must be in accordance with portable tank special provision TP3. Solids meeting the definition of an elevated temperature material must be transported in accordance with the applicable requirements of this subchapter.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 153
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 213
DOT Packaging Bulk (49 CFR 173.xxx)	: 240
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 100 kg
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 200 kg
DOT Vessel Stowage Location	: A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel.
DOT Vessel Stowage Other	: 52 - Stow "separated from" acids
<b>TDG</b>	
UN-No. (TDG)	: UN3439
TDG Special Provisions	: 16 - 1) The technical name of the most dangerous substance related to the primary class must be shown, in parentheses, on the shipping document following the shipping name in accordance with clause 3.5(1)(c)(i)(A) of Part 3, Documentation. The technical name must also be shown, in parentheses, on a small means of containment or on a tag following the shipping name in accordance with subsections 4.11(2) and (3) of Part 4, Dangerous Goods Safety Marks. 2) subsection (1), the technical name for the following dangerous goods is not required to be shown on a shipping document or on a small means of containment when Canadian law for domestic transport or an international convention for international transport prohibits the disclosure of the technical: a) UN1544, ALKALOID SALTS, SOLID, N.O.S. or ALKALOIDS, SOLID, N.O.S; b) UN1851, MEDICINE, LIQUID, TOXIC, N.O.S; c) UN3140, ALKALOID SALTS, LIQUID, N.O.S. or ALKALOIDS, LIQUID, N.O.S; d) UN3248, MEDICINE, LIQUID, FLAMMABLE, TOXIC, N.O.S; or e) UN3249, MEDICINE, SOLID, TOXIC, N.O.S. An example in Canada is the "Food and Drugs Act".
Explosive Limit and Limited Quantity Index	: 5 kg
Excepted quantities (TDG)	: E1
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index	: 100 kg
Emergency Response Guide (ERG) Number	: 151
<b>IMDG</b>	
Special provision (IMDG)	: 223, 274
Limited quantities (IMDG)	: 5 kg
Excepted quantities (IMDG)	: E1
Packing instructions (IMDG)	: P002, LP02
IBC packing instructions (IMDG)	: IBC08
IBC special provisions (IMDG)	: B3
Tank instructions (IMDG)	: T1



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Tank special provisions (IMDG)	: TP33
EmS-No. (Fire)	: F-A - FIRE SCHEDULE Alfa - GENERAL FIRE SCHEDULE
EmS-No. (Spillage)	: S-A - SPILLAGE SCHEDULE Alfa - TOXIC SUBSTANCES
Stowage category (IMDG)	: A
Segregation (IMDG)	: SG35
Properties and observations (IMDG)	: Solid, evolving toxic vapours. Reacts with acids or acid fumes, evolving hydrogen cyanide, a highly toxic and flammable gas. Soluble in water. Toxic if swallowed, by skin contact or by inhalation.

### IATA

PCA Excepted quantities (IATA)	: E1
PCA Limited quantities (IATA)	: Y645
PCA limited quantity max net quantity (IATA)	: 10kg
PCA packing instructions (IATA)	: 670
PCA max net quantity (IATA)	: 100kg
CAO packing instructions (IATA)	: 677
CAO max net quantity (IATA)	: 200kg
Special provision (IATA)	: A3, A5
ERG code (IATA)	: 6L

### 14.7. Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

All components of this product are present and listed as Active on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory, except for:

4-(Trifluoromethyl)benzonitrile	CAS-No. 455-18-5	100%
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### 15.2. International regulations

#### CANADA

#### 4-(Trifluoromethyl)benzonitrile (455-18-5)

Listed on the Canadian NDSL (Non-Domestic Substances List)

#### EU-Regulations

#### 4-(Trifluoromethyl)benzonitrile (455-18-5)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

#### National regulations

#### 4-(Trifluoromethyl)benzonitrile (455-18-5)

Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Japanese Poisonous and Deleterious Substances Control Law  
Listed on NZIoC (New Zealand Inventory of Chemicals)  
Listed on the Japanese ISHL (Industrial Safety and Health Law)  
Listed on the TCSI (Taiwan Chemical Substance Inventory)  
Listed on the NCI (Vietnam - National Chemical Inventory)

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### 15.3. US State regulations

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

### SECTION 16: Other information

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#### Full text of H-phrases

H301	Toxic if swallowed
H311	Toxic in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H332	Harmful if inhaled
H335	May cause respiratory irritation

NFPA health hazard

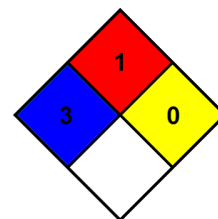
: 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA fire hazard

: 1 - Materials that must be preheated before ignition can occur.

NFPA reactivity

: 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health

: 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given

Flammability

: 1 Slight Hazard - Materials that must be preheated before ignition will occur. Includes liquids, solids and semi solids having a flash point above 200 F. (Class IIIB)

Physical

: 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Safety Data Sheet (SDS), USA

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is offered solely for your consideration, investigation, and verification. It does not represent any guarantee of the properties of the product nor that the hazard precautions or procedures described are the only ones which exist. SynQuest shall not be held liable for any damage resulting from handling or from contact with the above product.