

**1. PRODUCT AND COMPANY IDENTIFICATION**

Product name : 2-(Trifluoromethyl)benzotrile  
Product Number : 232947  
Brand : Aldrich  
Company : Sigma-Aldrich  
3050 Spruce Street  
SAINT LOUIS MO 63103  
USA  
Telephone : +18003255832  
Fax : +18003255052  
Emergency Phone # : (314) 776-6555

**2. COMPOSITION/INFORMATION ON INGREDIENTS**

Synonyms :  $\alpha,\alpha,\alpha$ -Trifluoro-o-tolunitrile  
Formula :  $C_8H_4F_3N$   
Molecular Weight : 171.12 g/mol

CAS-No.	EC-No.	Index-No.	Concentration
<b><math>\alpha,\alpha,\alpha</math>-Trifluoro-2-toluonitrile</b>			
447-60-9	207-184-3	-	-

**3. HAZARDS IDENTIFICATION****Emergency Overview****OSHA Hazards**

Combustible Liquid, Harmful by ingestion.

**HMIS Classification**

Health Hazard: 1  
Flammability: 2  
Physical hazards: 0

**NFPA Rating**

Health Hazard: 1  
Fire: 2  
Reactivity Hazard: 0

**Potential Health Effects**

**Inhalation** May be harmful if inhaled. May cause respiratory tract irritation.  
**Skin** May be harmful if absorbed through skin. May cause skin irritation.  
**Eyes** May cause eye irritation.  
**Ingestion** Harmful if swallowed.

#### 4. FIRST AID MEASURES

**General advice**

Consult a physician. Show this safety data sheet to the doctor in attendance. Move out of dangerous area.

**If inhaled**

If breathed in, move person into fresh air. If not breathing give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

#### 5. FIRE-FIGHTING MEASURES

**Flammable properties**

Flash point 90 °C (194 °F) - closed cup

Ignition temperature no data available

**Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**Special protective equipment for fire-fighters**

Wear self contained breathing apparatus for fire fighting if necessary.

#### 6. ACCIDENTAL RELEASE MEASURES

**Personal precautions**

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation.

**Environmental precautions**

Do not let product enter drains. Discharge into the environment must be avoided.

**Methods for cleaning up**

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

#### 7. HANDLING AND STORAGE

**Handling**

Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

**Storage**

Keep container tightly closed in a dry and well-ventilated place.

#### 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Contains no substances with occupational exposure limit values.

**Personal protective equipment****Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Hand protection**

Handle with gloves. For prolonged or repeated contact use protective gloves.

**Eye protection**

Safety glasses

**Skin and body protection**

Choose body protection according to the amount and concentration of the dangerous substance at the work place.

**Hygiene measures**

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

**9. PHYSICAL AND CHEMICAL PROPERTIES****Appearance**

Form liquid

**Safety data**

pH no data available

Melting point 7.5 °C (45.5 °F)

Boiling point no data available

Flash point 90 °C (194 °F) - closed cup

Ignition temperature no data available

Lower explosion limit no data available

Upper explosion limit no data available

Density 1.294 g/mL at 25 °C (77 °F)

Water solubility no data available

Partition coefficient: log Pow: 2.547  
n-octanol/water

**10. STABILITY AND REACTIVITY****Storage stability**

Stable under recommended storage conditions.

**Materials to avoid**

Strong oxidizing agents

**Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides, nitrogen oxides (NOx), Hydrogen fluoride

**11. TOXICOLOGICAL INFORMATION****Acute toxicity**

no data available

**Irritation and corrosion**

no data available

**Sensitisation**

Prolonged or repeated exposure may cause allergic reactions in certain sensitive individuals. The preceding data, or interpretation of data, was determined using Quantitative Structure Activity Relationship (QSAR) modeling.

#### Chronic exposure

- IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.
- ACGIH: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.
- NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

#### Signs and Symptoms of Exposure

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

#### Potential Health Effects

<b>Inhalation</b>	May be harmful if inhaled. May cause respiratory tract irritation.
<b>Skin</b>	May be harmful if absorbed through skin. May cause skin irritation.
<b>Eyes</b>	May cause eye irritation.
<b>Ingestion</b>	Harmful if swallowed.

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## 12. ECOLOGICAL INFORMATION

#### Elimination information (persistence and degradability)

no data available

#### Ecotoxicity effects

Toxicity to fish LC50 - Pimephales promelas (fathead minnow) - 42.2 mg/l - 96 h

#### Further information on ecology

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

no data available

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## 13. DISPOSAL CONSIDERATIONS

#### Product

This combustible material may be burned in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations. Contact a licensed professional waste disposal service to dispose of this material.

#### Contaminated packaging

Dispose of as unused product.

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## 14. TRANSPORT INFORMATION

#### DOT (US)

UN-Number: 3276 Class: 6.1

Packing group: III

Proper shipping name: Nitriles, toxic, liquid, n.o.s. ( $\alpha,\alpha,\alpha$ -Trifluoro-2-toluonitrile)

Marine pollutant: No

Poison Inhalation Hazard: No

**IMDG**

UN-Number: 3276 Class: 6.1 Packing group: III EMS-No: F-A, S-A  
Proper shipping name: NITRILES, TOXIC, LIQUID, N.O.S. ( $\alpha,\alpha,\alpha$ -Trifluoro-2-toluonitrile)  
Marine pollutant: No

**IATA**

UN-Number: 3276 Class: 6.1 Packing group: III  
Proper shipping name: Nitriles, toxic, liquid n.o.s. ( $\alpha,\alpha,\alpha$ -Trifluoro-2-toluonitrile)

**15. REGULATORY INFORMATION**

**OSHA Hazards**

Combustible Liquid, Harmful by ingestion.

**DSL Status**

This product contains the following components that are not on the Canadian DSL nor NDSL lists.

$\alpha,\alpha,\alpha$ -Trifluoro-2-toluonitrile	CAS-No. 447-60-9
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**SARA 302 Components**

SARA 302: No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

**SARA 313 Components**

SARA 313: This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

**SARA 311/312 Hazards**

Fire Hazard, Acute Health Hazard

**Massachusetts Right To Know Components**

No components are subject to the Massachusetts Right to Know Act.

**Pennsylvania Right To Know Components**

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**New Jersey Right To Know Components**

$\alpha,\alpha,\alpha$ -Trifluoro-2-toluonitrile	CAS-No. 447-60-9	Revision Date
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**California Prop. 65 Components**

This product does not contain any chemicals known to State of California to cause cancer, birth, or any other reproductive defects.

**16. OTHER INFORMATION**

**Further information**

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