

2-(Trifluoromethyl)thiophenol

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
SDS ID: 5861312
Issue date: 5/20/2025 Version: 1.0

SECTION 1: Identification

1.1. Identification

Product form	: Substance
Substance name	: 2-(Trifluoromethyl)thiophenol
CAS-No.	: 13333-97-6
Product code	: 5861-3-12
Formula	: C7H5F3S
Synonyms	: 2-Mercaptobenzotrifluoride; 2-(Trifluoromethyl)benzenethiol; 2-(Trifluoromethyl)phenyl mercaptan
Other means of identification	: MFCD00068896

1.2. Recommended use and restrictions on use

Use of the substance/mixture	: Laboratory chemicals Manufacture of substances Scientific research and development
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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 - www.synquestlabs.com

1.4. Emergency telephone number

Emergency number	: (844) 523-4086 (3E Company - Account 10069)
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SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS US classification

Flammable liquids Category 4	H227	Combustible liquid
Acute toxicity (oral) Category 3	H301	Toxic if swallowed
Acute toxicity (dermal) Category 3	H311	Toxic in contact with skin
Acute toxicity (inhalation:vapor) Category 3	H331	Toxic 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

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Hazard statements (GHS US)	: H227 - Combustible liquid H301+H311+H331 - Toxic if swallowed, in contact with skin or if inhaled H315 - Causes skin irritation H319 - Causes serious eye irritation H335 - May cause respiratory irritation
Precautionary statements (GHS US)	: P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking. 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. P311 - Call a POISON CENTER or doctor/physician 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. P370+P378 - In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish P403+P233 - Store in a well-ventilated place. Keep container tightly closed. P403+P235 - Store in a well-ventilated place. Keep cool. 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

Other hazards which do not result in classification : Stench.

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
2-(Trifluoromethyl)thiophenol (Main constituent)	CAS-No.: 13333-97-6	≤ 100	Flam. Liq. 4, H227 Acute Tox. 3 (Oral), H301 Acute Tox. 3 (Dermal), H311 Acute Tox. 3 (Inhalation:vapour), H331 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

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

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3.2. Mixtures

Not applicable

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. Sulfur oxides.
Explosion hazard	: Risk of explosion if heated under confinement. Use water spray or fog for cooling exposed containers.

5.3. Special protective equipment and precautions for fire-fighters

Firefighting instructions	: In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.
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 gas, fumes, vapor or spray.
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6.1.1. For non-emergency personnel

Emergency procedures	: Only qualified personnel equipped with suitable protective equipment may intervene.
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6.1.2. For emergency responders

Protective equipment	: Do not attempt to take action without suitable protective equipment. For further information refer to section 8: "Exposure controls/personal protection".
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Emergency procedures : Gas/vapor heavier than air. May accumulate in confined spaces, particularly at or below ground level.

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. Dike for recovery or absorb with appropriate material.
Methods for cleaning up : Take up large spills with pump or vacuum and finish with dry chemical absorbent. Use explosion-proof equipment. Take up small spills with dry chemical absorbent. Sweep or shovel spills into appropriate container for disposal. Ventilate area.
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 fumes, mist, spray, vapors. 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. Air sensitive. Keep contents under inert gas.
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

Appropriate engineering controls : Ensure good ventilation of the work station. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

8.3. Individual protection measures/Personal protective equipment

Hand protection:

protective gloves. 29 CFR 1910.138: Hand Protection

Eye protection:

Chemical goggles or safety glasses. Face shield. 29 CFR 1910.133: Eye and Face Protection

Skin and body protection:

Wear suitable protective clothing

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Respiratory protection:

In case of inadequate ventilation wear respiratory protection. 29 CFR 1910.134: Respiratory Protection

Personal protective equipment symbol(s):



Other information:

Safety shoes. 29 CFR 1910.136: Foot Protection.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Color	: No data available
Odor	: Stench
Odor threshold	: No data available
pH	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: 50 – 52 °C (@ 15 mm Hg)
Flash point	: 68 °C
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	: 1.35 g/ml
Molecular mass	: 178.17 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	: 1.499
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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.

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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

Strong oxidizing agents.

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)	: Inhalation:vapor: Toxic if inhaled.
Skin corrosion/irritation	: Causes skin irritation.
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

2-(Trifluoromethyl)thiophenol (13333-97-6)

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

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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	: UN2810
UN-No. (TDG)	: UN2810
UN-No. (IMDG)	: 2810
UN-No. (IATA)	: 2810

14.2. UN proper shipping name

Proper Shipping Name (DOT)	: Toxic, liquids, organic, n.o.s.
Proper Shipping Name (TDG)	: TOXIC LIQUID, ORGANIC, N.O.S.
Proper Shipping Name (IMDG)	: TOXIC LIQUID, ORGANIC, N.O.S.
Proper Shipping Name (IATA)	: Toxic liquid, organic, 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

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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.
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14.6. Special precautions for user

DOT

UN-No.(DOT)	: UN2810
DOT Special Provisions (49 CFR 172.102)	: IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). T7 - 4 178.274(d)(2) Normal..... 178.275(d)(3) TP1 - The maximum degree of filling must not exceed the degree of filling determined by the following: Degree of filling = $97 / 1 + a (tr - tf)$ Where: tr is the maximum mean bulk temperature during transport, and tf is the temperature in degrees celsius of the liquid during filling. TP28 - A portable tank having a minimum test pressure of 2.65 bar (265 kPa) may be used provided the calculated test pressure is 2.65 bar or less based on the MAWP of the hazardous material, as defined in 178.275 of this subchapter, where the test pressure is 1.5 times the MAWP.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 153
DOT Packaging Non Bulk (49 CFR 173.xxx)	: 203
DOT Packaging Bulk (49 CFR 173.xxx)	: 241
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 60 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 220 L
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	: 40 - Stow "clear of living quarters"

TDG

UN-No. (TDG)	: UN2810
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".

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Explosive Limit and Limited Quantity Index : 5 L
Excepted quantities (TDG) : E1
Passenger Carrying Road Vehicle or Passenger : 60 L
Carrying Railway Vehicle Index
Emergency Response Guide (ERG) Number : 153

IMDG

Special provision (IMDG) : 223, 274
Limited quantities (IMDG) : 5 L
Excepted quantities (IMDG) : E1
Packing instructions (IMDG) : P001, LP01
IBC packing instructions (IMDG) : IBC03
Tank instructions (IMDG) : T7
Tank special provisions (IMDG) : TP1, TP28
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
Stowage and handling (IMDG) : SW2
Properties and observations (IMDG) : Toxic if swallowed, by skin contact or by inhalation.

IATA

PCA Excepted quantities (IATA) : E1
PCA Limited quantities (IATA) : Y642
PCA limited quantity max net quantity (IATA) : 2L
PCA packing instructions (IATA) : 655
PCA max net quantity (IATA) : 60L
CAO packing instructions (IATA) : 663
CAO max net quantity (IATA) : 220L
Special provision (IATA) : A3, A4, A137
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:

2-(Trifluoromethyl)thiophenol	CAS-No. 13333-97-6	100%
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15.2. International regulations

CANADA

No additional information available

EU-Regulations

No additional information available

National regulations

No additional information available

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

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SECTION 16: Other information

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Full text of H-phrases	
H227	Combustible liquid
H301	Toxic if swallowed
H311	Toxic in contact with skin
H315	Causes skin irritation
H319	Causes serious eye irritation
H331	Toxic if inhaled
H335	May cause respiratory irritation

NFPA health hazard

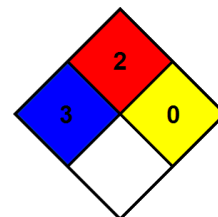
: 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA fire hazard

: 2 - Materials that must be moderately heated or exposed to relatively high ambient temperatures 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

: 2 Moderate Hazard - Materials which must be moderately heated or exposed to high ambient temperatures before ignition will occur. Includes liquids having a flash point at or above 100 F but below 200 F. (Classes II IIIA)

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 or any damage resulting from handling or from contact with the above product.