

## Safety Data Sheet 6662374

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Date of issue: 12/10/2015 Revision date: 01/26/2017 Version: 1.1

## **SECTION 1: Identification**

### Identification

Product form : Substance

Substance name 4-(Trifluoromethoxy)thiophenol

CAS No 169685-29-4 Product code 6662-3-74 Formula C7H5F3OS

Synonyms : 4-(Trifluoromethyoxy)benzenethiol

Other means of identification : MFCD00052312

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

: Laboratory chemicals Use of the substance/mixture

Manufacture of substances

Scientific research and development

### Details of the supplier of the safety data sheet

SynQuest Laboratories, Inc.

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### **Emergency telephone number**

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

## SECTION 2: Hazard(s) identification

## Classification of the substance or mixture

### Classification (GHS-US)

Acute Tox. 4 (Oral) H302 - Harmful if swallowed Acute Tox. 4 (Dermal) H312 - Harmful in contact with skin

Acute Tox. 3 (Inhalation) H331 - Toxic if inhaled Skin Irrit. 2 H315 - Causes skin irritation Eye Irrit. 2A H319 - Causes serious eye irritation STOT SE 3 H335 - May cause respiratory irritation

Full text of H-phrases: see section 16

## Label elements

## **GHS-US** labeling

Hazard pictograms (GHS-US)





: Danger

Signal word (GHS-US)

Hazard statements (GHS-US) H302+H312 - Harmful if swallowed or in contact with skin

H315 - Causes skin irritation H319 - Causes serious eye irritation

H331 - Toxic if inhaled

H335 - May cause respiratory irritation

: P261 - Avoid breathing fumes, mist, spray, vapors Precautionary statements (GHS-US)

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+P312 - If swallowed: Call a POISON CENTER or doctor/ physician if you feel unwell

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

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P312 - Call a POISON CENTER or doctor/physician if you feel unwell

P321 - Specific treatment (see supplemental first aid instructions 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 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

#### Other hazards 2.3.

Other hazards not contributing to the classification

: Stench.

## **Unknown acute toxicity (GHS US)**

Not applicable

## **SECTION 3: Composition/information on ingredients**

#### Substance

Substance type : Mono-constituent

Name	Product identifier	%	Classification (GHS-US)
4-(Trifluoromethoxy)thiophenol (Main constituent)	(CAS No) 169685-29-4	<= 100	Acute Tox. 4 (Oral), H302 Acute Tox. 4 (Dermal), H312 Acute Tox. 3 (Inhalation), H331 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

Full text of H-phrases: see section 16

#### **Mixture**

Not applicable

## **SECTION 4: First aid measures**

### **Description of first aid measures**

: In case of accident or if you feel unwell, seek medical advice immediately (show the label First-aid measures general

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.

Immediately flush eyes thoroughly with water for at least 15 minutes. Remove contact lenses, if First-aid measures after eye contact

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.

## Most important symptoms and effects, both acute and delayed

Symptoms/injuries The most important known symptoms and effects are described in the labelling (see section

2.2) and/or in section 11.

## Indication of any immediate medical attention and special treatment needed

Treat symptomatically.

## **SECTION 5: Firefighting measures**

### **Extinguishing media**

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media

appropriate for surrounding fire.

### Special hazards arising from the substance or mixture

Fire hazard : Thermal decomposition generates: Carbon oxides. Hydrogen fluoride. Sulfur oxides.

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

containers.

## **Advice for firefighters**

Firefighting instructions : In case of fire: Evacuate area. Fight fire remotely due to the risk of explosion.

Wear gas tight chemically protective clothing in combination with self contained breathing Protection during firefighting

apparatus. For further information refer to section 8: "Exposure controls/personal protection".

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### **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.

6.1.1. For non-emergency personnel

Emergency procedures : Only qualified personnel equipped with suitable protective equipment may intervene.

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".

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. Exposure 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.

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.

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

Protection.

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 : No data available
Odor threshold : No data available

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рΗ : No data available : No data available Melting point Freezing point : No data available Boiling point 64 - 66 (@ 15 mm Hg) Flash point No data available Relative evaporation rate (butyl acetate=1) : No data available Flammability (solid, gas) : No data available **Explosion limits** : No data available No data available Explosive properties : No data available Oxidizing properties Vapor pressure : No data available Relative density : No data available Relative vapor density at 20 °C : No data available · 194 17

Molecular mass

Solubility : No data available Log Pow No data available : No data available Auto-ignition temperature Decomposition temperature : No data available Viscosity : No data available Viscosity, kinematic : No data available Viscosity, dynamic : No data available

Other information

Refractive index : 1.4745 (@ 20 °C)

## **SECTION 10: Stability and reactivity**

## 10.1. Reactivity

No additional information available

## **Chemical stability**

The product is stable at normal handling and storage conditions.

## Possibility of hazardous reactions

No additional information available

## **Conditions to avoid**

No additional information available

### Incompatible materials

Air. Strong oxidizing agents.

## **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**

## Information on toxicological effects

Acute toxicity : Oral: Harmful if swallowed. Dermal: Harmful in contact with skin. Inhalation: Toxic if inhaled.

Skin corrosion/irritation Causes skin irritation. Serious eye damage/irritation Causes serious eye irritation.

: Not classified Respiratory or skin sensitization Germ cell mutagenicity : Not classified : Not classified Carcinogenicity Reproductive toxicity : Not classified

Specific target organ toxicity (single exposure) : May cause respiratory irritation.

Specific target organ toxicity (repeated : Not classified

exposure)

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Aspiration hazard : Not classified

## **SECTION 12: Ecological information**

#### **Toxicity**

No additional information available

## Persistence and degradability

No additional information available

## **Bioaccumulative potential**

No additional information available

#### Mobility in soil

No additional information available

#### Other adverse effects

No additional information available

## **SECTION 13: Disposal considerations**

### Waste treatment methods

Waste treatment methods : Remove to an authorized incinerator equipped with an afterburner and a flue gas scrubber. Waste 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**

## **Department of Transportation (DOT)**

In accordance with DOT

Transport document description : UN2810 Toxic, liquids, organic, n.o.s., 6.1, III

UN-No.(DOT) : UN2810

Proper Shipping Name (DOT) : Toxic, liquids, organic, n.o.s.

: 6.1 - Class 6.1 - Poisonous materials 49 CFR 173.132 Transport hazard class(es) (DOT)

Hazard labels (DOT) 6.1 - Poison



Packing group (DOT) : III - Minor Danger

DOT Packaging Non Bulk (49 CFR 173.xxx) : 203 DOT Packaging Bulk (49 CFR 173.xxx)

**DOT Symbols** : G - Identifies PSN requiring a technical name

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 - 4 178.27 $\dot{4}$ (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) DOT Quantity Limitations Passenger aircraft/rail : 60 L (49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 220 L

CFR 175.75)

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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"

Other information : No supplementary information available.

**TDG** 

No additional information available

Transport by sea

UN-No. (IMDG) : 2810

Proper Shipping Name (IMDG) : TOXIC LIQUID, ORGANIC, N.O.S.

Class (IMDG) : 6.1 - Toxic substances

Packing group (IMDG) : III - substances presenting low danger

Air transport

UN-No. (IATA) : 2810

Proper Shipping Name (IATA) : Toxic liquid, organic, n.o.s.

Class (IATA) : 6.1 - Toxic Substances

Packing group (IATA) : III - Minor Danger

## **SECTION 15: Regulatory information**

## 15.1. US Federal regulations

All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory except for:

4-(Trifluoromethoxy)thiophenol	CAS No 169685-29-4	100%
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This product or mixture does not contain a toxic chemical or chemicals in excess of the applicable de minimis concentration as specified in 40 CFR §372.38(a) subject to the reporting requirements of section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 and 40 CFR Part 372.

## 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 and/or reproductive harm

## **SECTION 16: Other information**

Revision date : 01/26/2017

## Full text of H-phrases:

Acute Tox. 3 (Inhalation)	Acute toxicity (inhalation) Category 3	
Acute Tox. 4 (Dermal)	Acute toxicity (dermal) Category 4	
Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4	
Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A	
Skin Irrit. 2	Skin corrosion/irritation Category 2	
STOT SE 3	Specific target organ toxicity (single exposure) Category 3	
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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NFPA health hazard : 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was

given

NFPA fire hazard : 1 - Must be preheated before ignition can occur.

NFPA reactivity : 1 - Normally stable, but can become unstable at elevated

temperatures and pressures or may react with water with

some release of energy, but not violently.



HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

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 : 1 Slight Hazard - Materials that are normally stable but can become unstable (self-react) at high

temperatures and pressures. Materials may react non-violently with water or undergo

hazardous polymerization in the absence of inhibitors.

SDS US (GHS HazCom 2012)

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.

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