# 4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride

## Safety Data Sheet

**Date of issue:** 08/16/2017  
**Version:** 1.0

### SECTION 1: Identification

#### 1.1. Identification

<table>
<thead>
<tr>
<th>Product form</th>
<th>Substance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Substance name</td>
<td>4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride</td>
</tr>
<tr>
<td>CAS No</td>
<td>947725-04-4</td>
</tr>
<tr>
<td>Product code</td>
<td>5771-3-01</td>
</tr>
<tr>
<td>Formula</td>
<td>C12H17F3S</td>
</tr>
<tr>
<td>Synonyms</td>
<td>[4-((1,1-Dimethylethyl)-2,6-dimethylyphenyl)[trifluorosulfur; 5-(tert-Butyl)-1,3-dimethyl-1-(trifluorothio)benzene; Fluolead</td>
</tr>
<tr>
<td>Other means of identification</td>
<td>MFCD11858620</td>
</tr>
</tbody>
</table>

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

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

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

**SynQuest Laboratories, Inc.**  
P.O. Box 309  
Alachua, FL 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

**Classification (GHS-US)**

- **Acute Tox. 3 (Oral):** H301 - Toxic if swallowed  
- **Acute Tox. 4 (Dermal):** H312 - Harmful in contact with skin  
- **Acute Tox. 4 (Inhalation):** H332 - Harmful if inhaled  
- **Skin Corr. 1B:** H314 - Causes severe skin burns and eye damage  
- **Eye Dam. 1:** H318 - Causes serious eye damage  
- **STOT SE 3:** H335 - May cause respiratory irritation

**Full text of H-phrases: see section 16**

#### 2.2. Label elements

**GHS-US labeling**

**Hazard pictograms (GHS-US):**

- GHS05  
- GHS06  
- GHS07

**Signal word (GHS-US):** Danger

**Hazard statements (GHS-US):**

- H301 - Toxic if swallowed  
- H312 + H332 - Harmful in contact with skin or if inhaled  
- H314 - Causes severe skin burns and eye damage  
- H335 - May cause respiratory irritation

**Precautionary statements (GHS-US):**

- P260 - Do not breathe dust, mist, spray  
- 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/doctor/…  
- P301 + P330 + P331 - If swallowed: rinse mouth. Do NOT induce vomiting  
- P302 + P352 - If on skin: Wash with plenty of soap and water  
- P303 + P361 + P353 - If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water/shower  
- P304 + P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing
4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride
Safety Data Sheet
according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P310 - Immediately call a POISON CENTER or doctor/physician
P321 - Specific treatment (see supplemental first aid instructions on this label)
P330 - Rinse mouth
P362+P364 - Take off contaminated clothing and wash it before reuse
P363 - Wash contaminated clothing 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
Other hazards not contributing to the classification: Reacts violently with water.

2.4. Unknown acute toxicity (GHS US)
Not applicable

SECTION 3: Composition/information on ingredients

3.1. Substance
Substance type: Mono-constituent

<table>
<thead>
<tr>
<th>Name</th>
<th>Product identifier</th>
<th>%</th>
<th>Classification (GHS-US)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride (Main constituent)</td>
<td>(CAS No) 947725-04-4</td>
<td>&lt;= 100</td>
<td>Acute Tox. 3 (Oral), H301</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Acute Tox. 4 (Dermal), H312</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Acute Tox. 4 (Inhalation), H332</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Skin Corr. 1B, H314</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Eye Dam. 1, H318</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>STOT SE 3, H335</td>
</tr>
</tbody>
</table>

Full text of H-phrases: see section 16

3.2. Mixture
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. Remove contaminated clothing and shoes. In case of skin contact, wearing rubber gloves rub 2.5% calcium gluconate gel continuously into the affected area for 1.5 hours or until further medical care is available. 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, 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.

Symptoms/injuries after inhalation: Material is destructive to tissue of the mucous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

4.3. Indication of any immediate medical attention and special treatment needed
Treat symptomatically. Absorption of excessive F- can result in acute systemic fluorosis with hypocalcemia, interference with various metabolic functions and organ damage (heart, liver, kidneys).

SECTION 5: Firefighting measures

5.1. Extinguishing media
Suitable extinguishing media: Dry powder. Use extinguishing media appropriate for surrounding fire.

5.2. Special hazards arising from the substance or mixture

5.3. Advice for firefighters
Firefighting instructions: In case of fire: Evacuate area.
### 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.

**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".

#### 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.

**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. Keep away from ignition sources. Keep contents under inert gas.

**Incompatible materials**: Refer to Section 10 on Incompatible Materials.

**Prohibitions on mixed storage**: Do not store with: Water.

**Storage area**: Store in dry, cool, well-ventilated area.

**Special rules on packaging**: Do not store in glass.

### 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.


**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.


### SECTION 9: Physical and chemical properties

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

**Physical state**: Solid

**Color**: No data available

**Odor**: No data available
4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride
Safety Data Sheet
according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
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<td>Flash point:</td>
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<td>Relative evaporation rate (butyl acetate=1)</td>
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<td>Flammability (solid, gas):</td>
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<td>Explosion limits:</td>
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<td>Explosive properties:</td>
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<td>Oxidizing properties:</td>
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<td>Decomposition temperature:</td>
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<td>Viscosity:</td>
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<tr>
<td>Viscosity, dynamic</td>
<td>No data available</td>
</tr>
</tbody>
</table>

9.2. Other information
No additional information available

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
Contact with acids liberates toxic gas. Contact with water liberates toxic gas.

10.4. Conditions to avoid
Keep away from heat, sparks and flame.

10.5. Incompatible materials

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. Dermal: Harmful in contact with skin. Inhalation: Harmful if inhaled.

Skin corrosion/irritation: Causes severe skin burns and eye damage.

Serious eye damage/irritation: Causes serious eye damage.

Respiratory or skin sensitization: Not classified

Germ cell mutagenicity: Not classified

Carcinogenicity: Not classified

Reproductive toxicity: Not classified

Specific target organ toxicity (single exposure): May cause respiratory irritation.
4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride
Safety Data Sheet
according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

Specific target organ toxicity (repeated exposure): Not classified
Aspiration hazard: Not classified
Potential Adverse human health effects and symptoms:
Absorption of excessive F- can result in acute systemic fluorosis with hypocalcemia, interference with various metabolic functions and organ damage (heart, liver, kidneys).
Symptoms/injuries after inhalation:
Material is destructive to tissue of the mucous membranes and upper respiratory tract. Cough, shortness of breath, headache, nausea.

SECTION 12: Ecological information

12.1. Toxicity
No additional information available

12.2. Persistence and degradability
No additional information available

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. 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: UN2923 Corrosive solids, toxic, n.o.s., 8, III
UN-No.(DOT): UN2923
Proper Shipping Name (DOT): Corrosive solids, toxic, n.o.s.
Transport hazard class(es) (DOT): 8 - Class 8 - Corrosive material 49 CFR 173.136
Hazard labels (DOT): 8 - Corrosive
6.1 - Poison

Packing group (DOT) III - Minor Danger
DOT Packaging Non Bulk (49 CFR 173.xxx) 213
DOT Packaging Bulk (49 CFR 173.xxx) 240
DOT Symbols: G - Identifies PSN requiring a technical name
4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride
Safety Data Sheet
according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations

DOT Special Provisions (49 CFR 172.102):
IB8 - Authorized IBCs: Metal (11A, 11B, 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 silt-proof and water-resistant or must be fitted with a silt-proof and water-resistant liner.

DOT Packaging Exceptions (49 CFR 173.xxx):

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27):
25 kg

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75):
100 kg

DOT Vessel Stowage Location:
B - (i) The material may be stowed “on deck” or “under deck” on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) “On deck only” on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.

DOT Vessel Stowage Other:
40 - Stow “clear of living quarters”, 95 - Stow “separated from” foodstuffs

Other information:
No supplementary information available.

TRANSPORT BY SEA

UN-NO. (IMDG):
2923

Proper Shipping Name (IMDG):
CORROSIVE SOLID, TOXIC, N.O.S.

Class (IMDG):
8 - Corrosive substances

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

AIR TRANSPORT

UN-NO. (IATA):
2923

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

Class (IATA):
8 - Corrosives

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-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride | CAS No 947725-04-4 | 100% |

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
4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride

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

National regulations

4-(tert-Butyl)-2,6-dimethylphenylsulfur trifluoride (947725-04-4)
Listed on the TCSI (Taiwan Chemical Substance Inventory)

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

Full text of H-phrases:

<table>
<thead>
<tr>
<th>Acute Tox. 3 (Oral)</th>
<th>Acute toxicity (oral) Category 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acute Tox. 4 (Dermal)</td>
<td>Acute toxicity (dermal) Category 4</td>
</tr>
<tr>
<td>Acute Tox. 4 (Inhalation)</td>
<td>Acute toxicity (inhalation) Category 4</td>
</tr>
<tr>
<td>Eye Dam. 1</td>
<td>Serious eye damage/eye irritation Category 1</td>
</tr>
<tr>
<td>Skin Corr. 1B</td>
<td>Skin corrosion/irritation Category 1B</td>
</tr>
<tr>
<td>STOT SE 3</td>
<td>Specific target organ toxicity (single exposure) Category 3</td>
</tr>
<tr>
<td>H301</td>
<td>Toxic if swallowed</td>
</tr>
<tr>
<td>H312</td>
<td>Harmful in contact with skin</td>
</tr>
<tr>
<td>H314</td>
<td>Causes severe skin burns and eye damage</td>
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<tr>
<td>H318</td>
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</tr>
<tr>
<td>H332</td>
<td>Harmful if inhaled</td>
</tr>
<tr>
<td>H335</td>
<td>May cause respiratory irritation</td>
</tr>
</tbody>
</table>

NFPA health hazard
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

NFPA fire hazard
: 0 - Materials that will not burn.

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
: 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is given
Flammability
: 0 Minimal Hazard - Materials that will not burn
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.