

### SECTION 1: Identification

#### 1.1. Identification

|                               |   |
|-------------------------------|---|
| Product form                  | : Substance   |
| Substance name                | : p-Tolyl trifluoromethanesulfonate                             |
| CAS No                        | : 29540-83-8  |
| Product code                  | : 6764-3-04   |
| Formula                       | : C <sub>8</sub> H <sub>7</sub> F <sub>3</sub> O <sub>3</sub> S |
| Synonyms                      | : 4-Methylphenyl triflate; p-Tolyl triflate                     |
| Other means of identification | : MFCD00192507  |

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

|                              |  |
|------------------------------|--|
| Use of the substance/mixture | : Laboratory chemicals<br>Manufacture of substances<br>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)

|                               |  |
|-------------------------------|--|
| Flam. Liq. 4                  | H227 - Combustible liquid                      |
| Acute Tox. 3 (Oral)           | H301 - Toxic if swallowed                      |
| Acute Tox. 3 (Dermal)         | H311 - Toxic in contact with skin              |
| Acute Tox. 3 (Inhalation:gas) | H331 - Toxic if inhaled                        |
| Skin Corr. 1C                 | H314 - Causes severe skin burns and eye damage |
| Eye Dam. 1                    | H318 - Causes serious eye damage               |
| Carc. 2                       | H351 - Suspected of causing cancer             |
| 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) :



Signal word (GHS-US) :

Danger

Hazard statements (GHS-US) :

H227 - Combustible liquid  
H301+H311+H331 - Toxic if swallowed, in contact with skin or if inhaled  
H314 - Causes severe skin burns and eye damage  
H335 - May cause respiratory irritation  
H351 - Suspected of causing cancer

Precautionary statements (GHS-US) :

P201 - Obtain special instructions before use  
P202 - Do not handle until all safety precautions have been read and understood  
P210 - Keep away from heat/sparks/open flames/hot surfaces. No smoking  
P260 - Do not breathe dust/fume/gas/mist/vapors/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/...

# p-Tolyl trifluoromethanesulfonate

## Safety Data Sheet

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

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  
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P308+P313 - If exposed or concerned: Get medical advice/attention  
P310 - Immediately call a POISON CENTER or doctor/ physician  
P311 - Call a POISON CENTER or doctor/physician  
P321 - Specific treatment (see supplemental first aid instructions on this label)  
P330 - Rinse mouth  
P361 - Take off immediately all contaminated clothing  
P363 - Wash contaminated clothing 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

No additional information available

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

Not applicable

## SECTION 3: Composition/information on ingredients

### 3.1. Substance

Substance type : Mono-constituent

| Name  | Product identifier  | %      | Classification (GHS-US)   |
|---|---------------------|--------|---|
| p-Tolyl trifluoromethanesulfonate<br>(Main constituent) | (CAS No) 29540-83-8 | <= 100 | Flam. Liq. 4, H227<br>Acute Tox. 3 (Oral), H301<br>Acute Tox. 3 (Dermal), H311<br>Acute Tox. 3 (Inhalation:gas),<br>H331<br>Skin Corr. 1C, H314<br>Eye Dam. 1, H318<br>Carc. 2, H351<br>STOT SE 3, H335 |

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. 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 mucuous 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.

# p-Tolyl trifluoromethanesulfonate

## Safety Data Sheet

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

### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media

Suitable extinguishing media : Alcohol resistant foam. Carbon dioxide. Dry powder. Water spray. Use extinguishing media appropriate for surrounding fire.

#### 5.2. Special hazards arising from the substance or mixture

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. May form flammable/explosive vapor-air mixture.

#### 5.3. Advice for firefighters

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.

##### 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. Consider the risk of potentially explosive atmospheres. Eliminate every possible source of ignition.

#### 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

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable.  
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. Keep away from ignition sources (including static discharges). Proper grounding procedures to avoid static electricity should be followed. Use only non-sparking tools.  
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.  
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

# p-Tolyl trifluoromethanesulfonate

## Safety Data Sheet

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

### 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    |
| pH  | : No data available    |
| Melting point                               | : No data available    |
| Freezing point                              | : No data available    |
| Boiling point                               | : 115 °C (@ 50 mm Hg)  |
| Flash point                                 | : 89 °C                |
| Relative evaporation rate (butyl acetate=1) | : No data available    |
| Flammability (solid, gas)                   | : No data available    |
| Explosion limits                            | : No data available    |
| Explosive properties                        | : No data available    |
| Oxidizing properties                        | : No data available    |
| Vapor pressure                              | : No data available    |
| Relative density                            | : No data available    |
| Relative vapor density at 20 °C             | : No data available    |
| Specific gravity / density                  | : 1.342 g/ml (@ 25 °C) |
| Molecular mass                              | : 240.2 g/mol          |
| Solubility                                  | : No data available    |
| Log Pow                                     | : No data available    |
| Auto-ignition temperature                   | : No data available    |
| Decomposition temperature                   | : No data available    |
| Viscosity                                   | : No data available    |
| Viscosity, kinematic                        | : No data available    |
| Viscosity, dynamic                          | : No data available    |

### 9.2. Other information

|                  |                   |
|------------------|-------------------|
| Refractive index | : 1.441 (@ 20 °C) |
|------------------|-------------------|

## 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

Strong acids. Strong bases. Strong oxidizing agents. Strong reducing agents.

# p-Tolyl trifluoromethanesulfonate

## Safety Data Sheet

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

### 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: Toxic in contact with skin. Inhalation:gas: Toxic if inhaled.

| p-Tolyl trifluoromethanesulfonate (29540-83-8) |                           |
|--|---------------------------|
| ATE US (oral)                                  | 100.000 mg/kg body weight |
| ATE US (dermal)                                | 300.000 mg/kg body weight |
| ATE US (gases)                                 | 700.000 ppmV/4h           |

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 : Suspected of causing cancer.  
Reproductive toxicity : Not classified  
Specific target organ toxicity (single exposure) : May cause respiratory irritation.  
Specific target organ toxicity (repeated exposure) : Not classified  
Aspiration hazard : Not classified  
Symptoms/injuries after inhalation : Material is destructive to tissue of the mucuous 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 : UN3265 Corrosive liquid, acidic, organic, n.o.s., 8, II

UN-No.(DOT) : UN3265

Proper Shipping Name (DOT) : Corrosive liquid, acidic, organic, n.o.s.

Transport hazard class(es) (DOT) : 8 - Class 8 - Corrosive material 49 CFR 173.136

# p-Tolyl trifluoromethanesulfonate

## Safety Data Sheet

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

Hazard labels (DOT) : 8 - Corrosive



Packing group (DOT) : II - Medium Danger

DOT Packaging Non Bulk (49 CFR 173.xxx) : 202

DOT Packaging Bulk (49 CFR 173.xxx) : 242

DOT Symbols : G - Identifies PSN requiring a technical name

DOT Special Provisions (49 CFR 172.102) : B2 - MC 300, MC 301, MC 302, MC 303, MC 305, and MC 306 and DOT 406 cargo tanks are not authorized.

IB2 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1). 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.

T11 - 6 178.274(d)(2) Normal..... 178.275(d)(3)

TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where:  $t_r$  is the maximum mean bulk temperature during transport,  $t_f$  is the temperature in degrees celsius of the liquid during filling, and  $a$  is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling ( $t_f$ ) and the maximum mean bulk temperature during transportation ( $t_r$ ) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where:  $d_{15}$  and  $d_{50}$  are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.

TP27 - A portable tank having a minimum test pressure of 4 bar (400 kPa) may be used provided the calculated test pressure is 4 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) : 154

DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27) : 1 L

DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75) : 30 L

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"

Other information : No supplementary information available.

### TDG

No additional information available

### Transport by sea

UN-No. (IMDG) : 3265

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

Class (IMDG) : 8 - Corrosive substances

Packing group (IMDG) : II - substances presenting medium danger

### Air transport

UN-No. (IATA) : 3265

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

Class (IATA) : 8 - Corrosives

Packing group (IATA) : II - Medium 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:

p-Tolyl trifluoromethanesulfonate

CAS No 29540-83-8

100%

# p-Tolyl trifluoromethanesulfonate

## Safety Data Sheet

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

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

##### p-Tolyl trifluoromethanesulfonate (29540-83-8)

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:

|                               |   |
|-------------------------------|---|
| Acute Tox. 3 (Dermal)         | Acute toxicity (dermal) Category 3                          |
| Acute Tox. 3 (Inhalation:gas) | Acute toxicity (inhalation:gas) Category 3                  |
| Acute Tox. 3 (Oral)           | Acute toxicity (oral) Category 3                            |
| Carc. 2                       | Carcinogenicity Category 2                                  |
| Eye Dam. 1                    | Serious eye damage/eye irritation Category 1                |
| Flam. Liq. 4                  | Flammable liquids Category 4                                |
| Skin Corr. 1C                 | Skin corrosion/irritation Category 1C                       |
| STOT SE 3                     | Specific target organ toxicity (single exposure) Category 3 |
| H227                          | Combustible liquid  |
| H301                          | Toxic if swallowed  |
| H311                          | Toxic in contact with skin                                  |
| H314                          | Causes severe skin burns and eye damage                     |
| H318                          | Causes serious eye damage                                   |
| H331                          | Toxic if inhaled  |
| H335                          | May cause respiratory irritation                            |
| H351                          | Suspected of causing cancer                                 |

NFPA health hazard

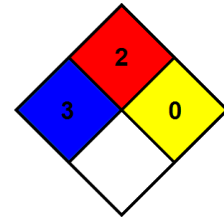
: 3 - Short exposure could cause serious temporary or residual injury even though prompt medical attention was given.

NFPA fire hazard

: 2 - Must be moderately heated or exposed to relatively high temperature before ignition can occur.

NFPA reactivity

: 0 - Normally stable, even under fire exposure conditions, and are not reactive with water.



HMIS III Rating

Health

: 2 Moderate Hazard - Temporary or minor injury may occur

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.

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.*