



TCI AMERICA

SAFETY DATA SHEET

Revision number: 1
Revision date: 10/06/2014

1. IDENTIFICATION

Product name: (3S,5R)-5-(2,4-Difluorophenyl)-5-[(1H-1,2,4-triazol-1-yl)methyl]oxolan-3-ylmethyl p-Toluenesulfonate
Product code: D4537

Product use: For laboratory research purposes.
Restrictions on use: Not for drug or household use.

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2. HAZARD(S) IDENTIFICATION

OSHA Haz Com: CFR 1910.1200: Not classifiable

Signal word: None

Hazard Statement(s): None

Pictogram(s) or Symbol(s): None

Precautionary Statement(s): None

Supplementary Information: While this material is not classified as hazardous under OSHA, this SDS contains valuable information critical to safe handling and proper use of the product. This SDS should be retained and available for employees and other users of this product.

3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance/Mixture: Substance
Components: (3S,5R)-5-(2,4-Difluorophenyl)-5-[(1H-1,2,4-triazol-1-yl)methyl]oxolan-3-ylmethyl p-Toluenesulfonate
Percent: >98.0%(HPLC)
CAS Number: 149809-43-8
Molecular Weight: 449.47
Chemical Formula: C₂₁H₂₁F₂N₃O₄S
Synonyms: p-Toluenesulfonic Acid (3S,5R)-5-(2,4-Difluorophenyl)-5-[(1H-1,2,4-triazol-1-yl)methyl]oxolan-3-ylmethyl Ester

4. FIRST-AID MEASURES

Inhalation: Move victim to fresh air. Call emergency medical service. Give artificial respiration if victim is not breathing. Administer oxygen if breathing is difficult. Keep victim warm and quiet. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.

Skin contact: Remove and isolate contaminated clothing and shoes. In case of contact with substance, immediately flush skin with running water for at least 20 minutes. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.

4. FIRST-AID MEASURES

| | |
|-------------------------------------|--|
| Eye contact: | Move victim to fresh air. Check for and remove any contact lenses. In case of contact with substance, immediately flush eyes with running water for at least 20 minutes. Keep victim warm and quiet. Treat symptomatically and supportively. Effects of exposure to substance may be delayed. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves. |
| Ingestion: | If a person vomits place them in the recovery position so that vomit will not reenter the mouth and throat. Rinse mouth. Keep victim warm and quiet. Loosen tight clothing such as a collar, tie, belt or waistband. If swallowed, seek medical advice immediately and show the container or label. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves. Effects of exposure (ingestion) to substance may be delayed. |
| Symptoms/effects: | |
| Acute: | No data available |
| Delayed: | No data available |
| Immediate medical attention: | If breathing has stopped, perform artificial respiration. Use first aid treatment according to the nature of the injury. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves. |

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media: Dry chemical, CO₂, water spray, or alcohol-resistant foam. Consult with local fire authorities before attempting large scale fire fighting operations.

Specific hazards arising from the chemical

Hazardous combustion products: These products include: Carbon oxides Nitrogen oxides Sulfur oxides Halogenated compounds
Other specific hazards: WARNING: Highly toxic HF gas is produced during combustion.

Special precautions for fire-fighters:

Not available

Special protective equipment for fire-fighters:

Structural fire fighters' protective clothing provides limited protection in fire situations ONLY; it may not be effective in spill situations.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions: Do not touch damaged containers or spilled material unless wearing appropriate protective clothing (Section 8).

Personal protective equipment: Wear protective clothing, gloves and eye protection.

Emergency procedures: In case of a spill and/or a leak, always shut off any sources of ignition, ventilate the area, and exercise caution.

Methods and materials for containment and cleaning up:

Dike far ahead of liquid spill for later disposal.

Environmental precautions:

Prevent entry into sewers, basements or confined areas.

7. HANDLING AND STORAGE

Precautions for safe handling: Provide appropriate exhaust ventilation at places where dust is formed. Normal measures for preventive fire protection. Follow safe industrial hygiene practices and always wear proper protective equipment when handling this compound.

Conditions for safe storage: Keep container tightly closed in a dry and well-ventilated place. Store under inert gas (e.g. Argon). Store in a freezer.

Storage incompatibilities: Store away from oxidizing agents

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Exposure limits: No data available

Appropriate engineering controls:

Good general ventilation should be sufficient to control airborne levels. Eyewash fountains should be provided in areas where there is any possibility that workers could be exposed to the substance. Follow safe industrial engineering/laboratory practices when handling any chemical.

Personal protective equipment

Respiratory protection: Dust respirator. Be sure to use a MSHA/NIOSH approved respirator or equivalent.

Hand protection: Wear protective gloves.

Eye protection: Safety glasses.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Skin and body protection: Lab coat.

9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state (20°C): Solid
Form: Crystal - Powder
Color: White - Pale yellow
Odor: No data available
Odor threshold: No data available

| | | | |
|--|-------------------|--|-------------------|
| Melting point/freezing point: | 107°C (225°F) | pH: | No data available |
| Boiling point/range: | No data available | Vapor pressure: | No data available |
| Decomposition temperature: | No data available | Vapor density: | No data available |
| Relative density: | No data available | Dynamic Viscosity: | No data available |
| Kinematic Viscosity: | No data available | | |
| Partition coefficient: n-octanol/water (log P _{ow}) | No data available | Evaporation rate: (Butyl Acetate = 1) | No data available |

| | | | |
|----------------------------|-------------------|-----------------------------------|-------------------|
| Flash point: | No data available | Autoignition temperature: | No data available |
| Flammability (solid, gas): | No data available | Flammability or explosive limits: | |
| | | Lower: | No data available |
| | | Upper: | No data available |

Solubility(ies):
Slightly soluble: Chloroform

10. STABILITY AND REACTIVITY

Reactivity: Not Available.
Chemical Stability: Stable under recommended storage conditions. (See Section 7)
Possibility of Hazardous Reactions: No hazardous reactivity has been reported.
Conditions to avoid: Exposure to air. Heat sensitive.
Incompatible materials: Oxidizing agents
Hazardous Decomposition Products: No data available

11. TOXICOLOGICAL INFORMATION

Acute Toxicity:
No data available

Skin corrosion/irritation:
No data available

Serious eye damage/irritation:
No data available

Respiratory or skin sensitization:
No data available

Germ cell mutagenicity:
No data available

Carcinogenicity:
No data available

IARC: No data available

NTP: No data available

OSHA: No data available

Reproductive toxicity:
No data available

Routes of Exposure: Inhalation, Eye contact, Ingestion.

Symptoms related to exposure:

No specific information is available in our data base regarding the toxic effects of this material for humans. However, exposure to any chemical should be kept to a minimum. Always follow safe industrial hygiene practices and wear proper protective equipment when handling this compound.

Potential Health Effects:

No specific information available; skin and eye contact may result in irritation. May be harmful if inhaled or ingested.

Target organ(s): No data available

12. ECOLOGICAL INFORMATION

Ecotoxicity

Fish: No data available
Crustacea: No data available
Algae: No data available

Persistence and degradability: No data available

Bioaccumulative potential (BCF): No data available

Mobility in soil: No data available

Partition coefficient: No data available

n-octanol/water (log P_{ow})

Soil adsorption (K_{oc}): No data available

Henry's Law: No data available

constant (PaM³/mol)

13. DISPOSAL CONSIDERATIONS

Disposal of product: Recycle to process if possible. It is the generator's responsibility to comply with Federal, State and Local rules and regulations. You may be able to dissolve or mix material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber system. This section is intended to provide assistance but does not replace these laws, nor does compliance in accordance with this section ensure regulatory compliance according to the law. US EPA guidelines for Identification and Listing of Hazardous Waste are listed in 40 CFR Parts 261.

Disposal of container: Dispose of as unused product.

Other considerations: Observe all federal, state and local regulations when disposing of the substance.

14. TRANSPORT INFORMATION

DOT (US) Non-hazardous for transportation.

IATA Non-hazardous for transportation.

IMDG Non-hazardous for transportation.

15. REGULATORY INFORMATION

Toxic Substance Control Act (TSCA 8b.):

This product is NOT on the EPA Toxic Substances Control Act (TSCA) inventory. The following notices are required by 40 CFR 720.36 (C) for those products not on the inventory list:

(i) These products are supplied solely for use in research and development by or under the supervision of a technically qualified individual as defined in 40 CFR 720.0 et sec.

(ii) The health risks of these products have not been fully determined. Any information that is or becomes available will be supplied on a SDS sheet.

US Federal Regulations

CERCLA Hazardous substance and Reportable Quantity:

SARA 313: Not Listed
SARA 302: Not Listed

State Regulations

State Right-to-Know

Massachusetts Not Listed
New Jersey Not Listed
Pennsylvania Not Listed
California Proposition 65: Not Listed

15. REGULATORY INFORMATION

Other Information

NFPA Rating:

Health: 0
Flammability: 0
Instability: 0

HMIS Classification:

Health: 0
Flammability: 0
Physical: 0

International Inventories

WHMIS hazard class: No data available.

16. OTHER INFORMATION

Revision date: 10/06/2014

Revision number: 1

TCI chemicals are for research purposes only and are NOT intended for use as drugs, food additives, household products, or pesticides. The information herein is believed to be correct, but does not claim to be all inclusive and should be used only as a guide. Neither the above named supplier nor any of its affiliates or subsidiaries assumes any liability whatsoever for the accuracy or completeness of the information contained herein. Final determination of suitability of any material is the sole responsibility of the user. All chemical reagents must be handled with the recognition that their chemical, physiological, toxicological, and hazardous properties have not been fully investigated or determined. All chemical reagents should be handled only by individuals who are familiar with their potential hazards and who have been fully trained in proper safety, laboratory, and chemical handling procedures. Although certain hazards are described herein, we can not guarantee that these are the only hazards which exist. Our SDS are based only on data available at the time of shipping and are subject to change without notice as new information is obtained. Avoid long storage periods since the product is subject to degradation with age and may become more dangerous or hazardous. It is the responsibility of the user to request updated SDS for products that are stored for extended periods. Disposal of unused product must be undertaken by qualified personnel who are knowledgeable in all applicable regulations and follow all pertinent safety precautions including the use of appropriate protective equipment (e.g. protective goggles, protective clothing, breathing equipment, face mask, fume hood). For proper handling and disposal, always comply with federal, state and local regulations.