

	lopentadienyl)zirconium(IV) uoromethanesulfonate)tetrahydrofuran x	Pricing >	
Zirconiu	um Trifluoromethanesulfonate	Pricing >	
Linear Formula	$C_{12}H_{10}F_6O_6S_2Zr \cdot C_4H_6O$		
Pubchem CID	16212672		
MDL Number	MFCD00192583		
EC No.	N/A		
IUPAC Name	cyclopentane; oxolane; trifluoromethanesulfonate; zirconium(2+)		
Beilstein/Reaxys No.	N/A		
	C1CCOC1.[CH]1[CH][CH][CH]1.[CH]1[CH][CH][CH][CH][CH][CH][CH]5.(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].Zr+2.(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)(F)(F)(F)S(=0)(=0)[0-].C(F)(F)(F)(F)(F)(F)(F)(F)(F)(F)(F)(F)(F)(		
SMILES		InChI=1\$/2C5H5.C4H8O.2CHF3O3\$.Zr/c3*1-2-4-5-3-1;2*2-1(3,4)8(5,6)7;/h2*1-5H;1-4H2;2*(H,5,6,7);/q;;;;;+2/p-2	
SMILES Inchl Identifier	InChI=1S/2C5H5.C4H8O.2CHF3O3S.Zr/c3*1-2-4-5-3-1;2*2-1(3,4)8(5,6)7;/h2*1-5H;1-4H2;2*(I	H,5,6,7);/q;;;;+2/p-2	

Inchl Key OFTAVORSNHLQHT-UHFFFAOYSA-L		
Signal Word	Warning	
Hazard Statements	H315-H319-H335	
Hazard Codes	Xi	
Risk Codes	36/37/38	
Safety Statements	16-26-36	
RTECS Number	N/A	
Transport Information	N/A	
WGK Germany	3	
GHS Pictograms	GHS07 Exclamation Point  CHS02 Flame	

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### **SAFETY DATA SHEET**

**Date Accessed:** 05/14/2024 **Date Revised:** 01/15/2022

### **SECTION 1. IDENTIFICATION**

**Product Identifiers:** All applicable American Elements product codes for CAS #89672-77-5

#### Relevant identified uses of the substance:

Scientific research and development

Supplier details: American Elements 10884 Weyburn Ave. Los Angeles, CA 90024 Tel: +1 310-208-0551 Fax: +1 310-208-0351

Emergency telephone number: Domestic, North America +1 800-424-9300 International +1 703-527-3887

#### **SECTION 2. HAZARDS IDENTIFICATION**

OSHA Haz Com: CFR 1910.1200: Skin Corrosion/Irritation [Category 2] Eye Damage/Irritation [Category 2A] Flammable Solids [Category 2] Signal word: Warning! Hazard Statement(s): Causes serious eye irritation Causes skin irritation Flammable solid





Pictogram(s) or Symbol(s):

Precautionary Statement(s):

[Prevention] Wash hands and face thoroughly after handling. Wear protective gloves. Wear eye and face protection.

Keep away from heat, sparks, open flames or other hot surfaces. - No smoking. Ground or bond container and receiving equipment. Use explosion-proof electrical, ventilating, lighting, and equipment. Wear protective gloves, eye protection and face protection. [Response] If on skin: Wash with plenty of water. If skin irritation or rash occurs: Get medical advice/attention. Take off

contaminated clothing and wash it before reuse. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. If eye irritation persists: Get medical advice or attention. In case of fire: Use dry chemical, CO2, sand, earth, water spray or regular foam to extinguish.

[Storage] None [Disposal] None

### SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance/Mixture: Substance Components: Zirconocene

Bis(trifluoromethanesulfonate) Tetrahydrofuran

Adduct

Percent: >97.0%(T)
CAS Number: 89672-77-5
Molecular Weight: 591.65

Chemical Formula: C16H18F6O7S2Zr Synonyms: Bis(cyclopentadienyl)zirconium Bis(trifluoromethanesulfonate) Tetrahydrofuran

Adduct, Zirconocene

Bis(triflate) Tetrahydrofuran Adduct

### **SECTION 4. FIRST AID MEASURES**

Inhalation: Call emergency medical service. Move victim to fresh air. 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: Call a poison center or doctor if you feel unwell. Remove and wash contaminated clothing before re-use. 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.

Eye contact: IMMEDIATELY flush eyes with running water for at least 15 minutes, keeping eyelids open. Contact with

material may irritate or burn eyes. Call emergency medical service. Move victim to fresh air. Check for and

remove any contact lenses. 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: Do not induce vomiting with out medical advice. If swallowed, seek medical advice immediately and show

the container or label. Do not use mouth-to-mouth method if victim ingested the substance; give artificial

respiration with the aid of a pocket mask equipped with a one-way valve or other proper respiratory medical device. Loosen tight clothing such as a collar, tie, belt or waistband. 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. Treat symptomatically and supportively. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves.

Symptoms/effects: Acute: Redness.

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.

### **SECTION 5. FIREFIGHTING MEASURES**

Suitable extinguishing media: Dry chemical, CO2, sand, earth, water spray or regular 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 Halogenated compounds Silicates Metallic oxides Other specific hazards: WARNING: Highly toxic HF gas is produced during combustion. Special precautions for fire-fighters: Use water spray or fog; do not use straight streams. Dike fire-control water for later disposal; do not scatter the material. May re-ignite after fire is extinguished. Runoff to sewer may create fire or explosion hazard. Containers may explode when heated. Move containers from fire area if you can do it without risk.

Special protective equipment for fire-fighters: Wear positive pressure self-contained breathing apparatus (SCBA). Structural fire fighters' protective clothing provides limited protection in fire situations ONLY; it may not be effective in spill situations. Wear chemical protective clothing which is specifically recommended by the manufacturer. It may provide little or no thermal protection.

#### **MEASURES**

Personal precautions: Avoid contact with skin, eyes, and clothing. Keep people away from and upwind of spill/leak. Use sparkproof

tools and explosion-proof equipment. Remove all sources of ignition. Do not touch damaged containers or spilled material unless wearing appropriate protective clothing (Section 8). Warn unnecessary personnel to move away. Stop leak if you can do it without risk. Ensure adequate ventilation.

Isolate the hazard area and deny entry to unnecessary and unprotected personnel.

Personal protective equipment: Wear eye protection (splash goggles) and face protection (full length face shield). Lab coat. Dust

respirator. Be sure to use a MSHA/NIOSH approved respirator or equivalent. Wear protective gloves (nitrile).

Emergency procedures: Prevent dust cloud. ELIMINATE all ignition sources (no smoking, flares, sparks or flames in the immediate area). Do not touch damaged containers or spilled material unless wearing appropriate protective clothing.

Warn personnel to move away. Prevent entry into sewers, basements or confined areas; dike if needed. Methods and materials for containment and cleaning up:

ELIMINATE all ignition sources (no smoking, flares, sparks, or flames in immediate area). All equipment used when handling the product must be grounded. Stop leak if without risk. Ventilate the area. Absorb with an inert material and put the spilled material in an appropriate waste disposal container. Use clean non-sparking tools to collect absorbed material.

Environmental precautions:

Prevent further leakage or spillage if safe to do so. Water runoff can cause environmental damage. Prevent entry into sewers, basements or confined areas; dike if needed.

#### SECTION 7. HANDLING AND STORAGE

Precautions for safe handling: Avoid inhalation of vapor or mist. Avoid contact with skin and eyes. Avoid mechanical shock and friction.

Avoid formation of dust and aerosols. Keep away from heat and sources of ignition. Use explosion-proof equipment. Use only non-sparking hand tool when handling this product. Ground all equipment

containing

material. Take measures to prevent build up of electrostatic charge. Good general ventilation should be

sufficient to control airborne levels. Keep container dry. Handle and open container with care. Wear suitable protective clothing, gloves and eye/face protection. When using do not eat, drink, or smoke. Keep

away from sources of ignition.

Conditions for safe storage: Keep containers tightly closed in a cool, well-ventilated place. Keep away from sources of ignition. Store

and use away from heat, sparks, open flame, or any other ignition source. Keep away from incompatibles. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Avoid prolonged storage periods. Store under inert gas (e.g. Argon). Hygroscopic material, store in a tightly sealed container.

Storage incompatibilities: Store away from oxidizing agents

### SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Exposure limits: No data available Appropriate engineering controls:

Good general ventilation should be sufficient to control airborne levels. Ventilation is normally required when handling or using this product. 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. Skin and body protection: Lab coat.

# SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Physical state (20°C): Solid Form: Crystal - Powder

Color: Pale yellow - Gravish yellow red

Odor: No data available

Odor threshold: No data available

Melting point/freezing point: No data available

Boiling point/range: No data available

Decomposition temperature: No data available

Relative density: No data available Kinematic Viscosity: No data available Partition coefficient: No data available

n-octanol/water (log Pow) Flash point: 79°C (174°F)

Flammability (solid, gas): No data available

pH: No data available

Vapor pressure: No data available Vapor density: No data available Dynamic Viscosity: No data available Evaporation rate: No data available

(Butyl Acetate = 1)

Autoignition temperature: No data available

Flammability or explosive limits: No data available

Lower: No data available Upper: No data available

Solubility(ies):

### SECTION 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: Avoid excessive heat and light. Incompatible materials: Acids, Alkali, Bases, Oxidizing

agents

Hazardous Decomposition Products: No data

available

### SECTION 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, Skin contact.

Symptoms related to exposure:

Skin contact may result in inflammation; characterized by itching, scaling, reddening, or occasionally blistering. Skin contact may result in redness, pain or dry skin. Eye contact may result in redness or pain.

Potential Health Effects:

Skin and eye contact may result in irritation.

Target organ(s): No data available

#### **SECTION 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

Mobillity in soil: No data available

Partition coefficient: n-octanol/water (log Pow) No data available

Soil adsorption (Koc): No data available

Henry's Law:

constant (PaM3/mol) No data available

# SECTION 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. The product should not be allowed to enter the environment, drains.

water ways, or the soil.

Disposal of container: Dispose of as unused product.

Do not re-use empty containers.

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

#### **SECTION 14. TRANSPORT INFORMATION**

DOT (US)

UN number:

UN1325

**Proper Shipping Name:** 

Flammable solids, organic, n.o.s.

Class or Division:

4.1 Flammable solid

Packing Group:

Ш

IATA

UN number:

UN1325

**Proper Shipping Name:** 

Flammable solids, organic, n.o.s.

Class or Division:

4.1 Flammable solid

Packing Group:

Ш

**IMDG** 

UN number:

UN1325

Proper Shipping Name:

Flammable solids, organic, n.o.s.

Class or Division:

4.1 Flammable solid

Packing Group:

Ш

EmS number: F-A, S-G

### SECTION 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

Other Information NFPA Rating: Health: 3 Flammability: 2

Flammability: 2 Instability: 0

HMIS Classification:

Health: 3 Flammability: 2 Physical: 0

International Inventories International Inventories

WHMIS hazard class: B4: Flammable Solid. D2B: Materials causing other toxic effects. (Toxic)

#### 16. OTHER INFORMATION

Safety Data Sheet according to Regulation (EC) No. 1907/2006 (REACH). 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 applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. American Elements shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale. COPYRIGHT 1997-2022 AMERICAN ELEMENTS. LICENSED GRANTED TO MAKE UNLIMITED PAPER COPIES FOR INTERNAL USE ONLY.