



<a href="#">Bis(pentamethylcyclopentadienyl)zirconium(IV) Dichloride</a>		<a href="#">Pricing &gt;</a>
Linear Formula	C <sub>20</sub> H <sub>30</sub> Cl <sub>2</sub> Zr	
Pubchem CID	16058028	
MDL Number	MFCD00058849	
EC No.	N/A	
IUPAC Name	dichlorozirconium(2+); 1,2,3,4,5-pentamethylcyclopenta-1,3iene	
SMILES	C[C-]1C(=C(C(=C1C)C)C)C.C.[C-]1C(=C(C(=C1C)C)C)C.Cl[Zr+2]Cl	
Inchl Identifier	InChI=1S/2C10H15.2ClH.Zr/c2*1-6-7(2)9(4)10(5)8(6)3;;;/h2*1-5H3;2*1H;/q2*-1;;;+4/p-2	
Inchl Key	UJYDWRDELGVHLP-UHFFFAOYSA-L	
Signal Word	Danger	
Hazard Statements	H261-H301-H311-H332-H314-H318	
Hazard Codes	Xn, C	
Risk Codes	14-20/21/22-34	
Safety Statements	26-36/37/39-45	
RTECS Number	N/A	
Transport Information	UN3096 8/PG II	
WGK Germany	N/A	
GHS Pictograms	<a href="#">GHS05 Corrosive</a>  <a href="#">GHS07 Exclamation Point</a> 	

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## SAFETY DATA SHEET

Date Accessed: 05/02/2024

Date Revised: 01/15/2022

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## SECTION 1. IDENTIFICATION

**Product Identifiers:** All applicable American Elements product codes for CAS #54039-38-2

**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

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## SECTION 2. HAZARDS IDENTIFICATION

OSHA Haz Com: CFR 1910.1200: Acute Toxicity - Oral [Category 4]  
Acute Toxicity - Dermal [Category 4]  
Acute Toxicity - Inhalation [Category 4]  
Eye Damage/Irritation [Category 1]  
Corrosive to Metals [Category 1]  
Skin Corrosion/Irritation [Category 1C]  
Signal word: Danger!  
Hazard Statement(s): Causes serious eye damage  
Causes severe skin burns and eye damage  
Harmful if swallowed  
Harmful in contact with skin  
Harmful if inhaled  
May be corrosive to metals



Pictogram(s) or Symbol(s):  
Precautionary Statement(s):  
[Prevention] Do not eat, drink or smoke when using this product. Wash hands and face thoroughly after handling. Wear protective gloves and protective clothing. Avoid breathing dusts or mists. Use only outdoors or in a wellventilated area. Do not breathe dusts or mists. Wear protective gloves, protective clothing, eye protection and face protection. Wear eye protection. Wear face protection (full length face shield). Keep only in

original container.

[Response] If swallowed: Immediately call a poison center or doctor. Rinse mouth. If on skin: Wash with plenty of water. Call a poison center or doctor if you feel unwell. Take off contaminated clothing and wash it before reuse. If inhaled: Remove person to fresh air and keep comfortable for breathing. If swallowed: Rinse mouth. Do NOT induce vomiting. If on skin (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower. Wash contaminated clothing before reuse. Immediately call a poison center or doctor. If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Absorb spillage to prevent material damage.

[Storage] Store locked up. Store in corrosive resistant container with a resistant inner liner.

[Disposal] Dispose of contents and container in accordance with US EPA guidelines for the classification and determination of hazardous waste listed in 40 CFR 261.3. (See Section 13)

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### **SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance/Mixture: Substance

Components: Decamethylzirconocene Dichloride

Percent: >98.0%(T)

CAS Number: 54039-38-2

Molecular Weight: 432.58

Chemical Formula: C<sub>20</sub>H<sub>30</sub>Cl<sub>2</sub>Zr

Synonyms:

Bis(pentamethylcyclopentadienyl)zirconium(IV)

Dichloride

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

Inhalation: Immediately call a poison center or doctor. Effects of exposure (inhalation) to substance may be delayed.

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: For severe burns, immediate medical attention is required. Immediately call a poison center or doctor.

Remove and wash contaminated clothing before re-use. 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.

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

Eye contact

with vapors or substance may cause severe injury, burns, or death. 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: Harmful if swallowed. Do not induce vomiting without medical advice. Call a physician or Poison Control

Center immediately. 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: Pain. Redness.

Delayed: No data available

Immediate medical attention: WARNING: It might be hazardous to the person providing aid to give mouth-to-mouth respiration, because

the inhaled material is harmful. WARNING: It might be hazardous to the person providing aid to give mouth-to-mouth respiration, because the inhaled material is corrosive. For severe burns, immediate medical attention is required. 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.

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## **SECTION 5. FIREFIGHTING MEASURES**

Suitable extinguishing media: Dry chemical, CO<sub>2</sub> or water spray. 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  
Metallic oxides

Other specific hazards: WARNING: Highly toxic HCl 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. 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.

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## **SECTION 6. ACCIDENTAL RELEASE MEASURES**

Personal precautions: Avoid contact with skin, eyes, and clothing. Keep people away from and upwind of spill/leak. 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. In case of a spill and/or a leak, always shut off any sources of ignition, ventilate the area, and exercise caution. 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). Stop leak if without risk. 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. Ventilate the area.

Environmental precautions:

Keep away from living quarters. 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.

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## **SECTION 7. HANDLING AND STORAGE**

Precautions for safe handling: Avoid inhalation of vapor or mist. Manipulate under an adequate fume hood. Do not ingest. Avoid contact with skin and eyes. Avoid contact with skin. May corrode metallic surfaces. 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: Store in corrosive resistant container with a resistant inner liner. Keep containers tightly closed in a cool, well-ventilated place. Store locked up. 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). Moisture sensitive.

Storage incompatibilities: Bases, Store away from oxidizing agents

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## **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: Nitrile gloves.

Eye protection: Safety glasses.

Skin and body protection: Lab coat.

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## **SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES**

Physical state (20°C): Solid

Form: Crystal - Powder

Color: Slightly pale yellow - Yellow

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: No data available

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):

Soluble: Pyridine

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## **SECTION 10. STABILITY AND REACTIVITY**

Reactivity: Corrodes in contact with metals.

Chemical Stability: Moisture sensitive.

Possibility of Hazardous Reactions: No hazardous reactivity has been reported.

Conditions to avoid: Exposure to moisture. Moisture

sensitive.

Incompatible materials: Oxidizing agents

Hazardous Decomposition Products: No data available

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## **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:

Overexposure may result in serious illness or death.

Skin contact may produce burns. Skin contact may result in inflammation; characterized by itching, scaling, reddening, or occasionally blistering. Eye contact can result in corneal damage or blindness.

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

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## **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

Mobility 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 (PaM<sup>3</sup>/mol)  
No data available

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## **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.

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## **SECTION 14. TRANSPORT INFORMATION**

DOT (US)  
UN number:  
UN1759  
Proper Shipping Name:  
Corrosive solids, n.o.s.  
Class or Division:  
8 Corrosive material  
Packing Group:  
III  
IATA  
UN number:  
UN1759  
Proper Shipping Name:  
Corrosive solids, n.o.s.  
Class or Division:  
8 Corrosive material  
Packing Group:  
III  
IMDG  
UN number:  
UN1759

Proper Shipping Name:  
Corrosive solids, n.o.s.  
Class or Division:  
8 Corrosive material  
Packing Group:  
III  
EmS number: F-A, S-B

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## **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: 2

Flammability: 0

Instability: 0

HMIS Classification:

Health: 2

Flammability: 0

Physical: 0

International Inventories

WHMIS hazard class: E: Corrosive material.

D2A: Materials causing other toxic effects. (Very Toxic)

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## **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.

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