# SECTION 1: Identification of the substance/mixture and of the company/undertaking

## 1.1. Product identifier

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Product form</td>
<td>Substance</td>
</tr>
<tr>
<td>Physical state</td>
<td>Solid</td>
</tr>
<tr>
<td>Substance name</td>
<td>ZIRCONIUM DIISOPROPOXIDE BIS(2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONATE), tech-90</td>
</tr>
<tr>
<td>Product code</td>
<td>AKZ948</td>
</tr>
<tr>
<td>Formula</td>
<td>C28H52O6Zr</td>
</tr>
<tr>
<td>Synonyms</td>
<td>DIISOPROPOXYZIRCONIUM TMHD</td>
</tr>
<tr>
<td>Chemical family</td>
<td>METAL ESTER</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Use of the substance/mixture</td>
<td>Chemical intermediate</td>
</tr>
<tr>
<td></td>
<td>For research use only</td>
</tr>
</tbody>
</table>

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

**GELEST, INC.**  
11 East Steel Road  
Morrisville, PA 19067  
USA  
T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST  
info@gelest.com - www.gelest.com  

**1.4. Emergency telephone number**  
Emergency number: CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)

# SECTION 2: Hazards identification

## 2.1. Classification of the substance or mixture

**GHS-US classification**  
Eye Irrit. 2A  
H319

Full text of H-phrases: see section 16

## 2.2. Label elements

**GHS-US labelling**  
Hazard pictograms (GHS-US)  
GHS07

Signal word (GHS-US)  
Warning

Hazard statements (GHS-US)  
P280 - Wear protective gloves/protective clothing/eye protection/face protection

Precautionary statements (GHS-US)  
P264 - Wash hands thoroughly after handling

P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

P337+P313 - If eye irritation persists: Get medical advice/attention

## 2.3. Other hazards

No additional information available

## 2.4. Unknown acute toxicity (GHS US)

No data available

# SECTION 3: Composition/Information on ingredients

## 3.1. Substance

<table>
<thead>
<tr>
<th>Attribute</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Substance type</td>
<td>Mono-constituent</td>
</tr>
<tr>
<td>Name</td>
<td>ZIRCONIUM DIISOPROPOXIDE BIS(2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONATE), tech-90</td>
</tr>
<tr>
<td>CAS No</td>
<td>204522-78-1</td>
</tr>
</tbody>
</table>
ZIRCONIUM DIISOPROPOXIDE BIS(2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONATE), tech-90
Safety Data Sheet

### Name
Zirconium diisoprooxide bis(2,2,6,6-tetramethyl-3,5-heptanedionate) (CAS No) 204522-78-1

<table>
<thead>
<tr>
<th>%</th>
<th>GHS-US classification</th>
</tr>
</thead>
<tbody>
<tr>
<td>95 - 100</td>
<td>Eye Irrit. 2A, H319</td>
</tr>
</tbody>
</table>

3.2. Mixture
Not applicable

### SECTION 4: First aid measures

#### 4.1. Description of first aid measures

**First-aid measures general**: Remove contaminated clothing and shoes. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible). If possible show this sheet; if not available show packaging or label.

**First-aid measures after inhalation**: Remove victim to fresh air and keep at rest in a position comfortable for breathing. If you feel unwell, seek medical advice.

**First-aid measures after skin contact**: Wash with plenty of soap and water. Get 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 medical advice/attention.

**First-aid measures after ingestion**: Never give anything by mouth to an unconscious person. Get medical advice/attention.

#### 4.2. Most important symptoms and effects, both acute and delayed

**Symptoms/injuries after inhalation**: May cause irritation to the respiratory tract.

**Symptoms/injuries after skin contact**: May cause skin irritation.

**Symptoms/injuries after eye contact**: Causes serious eye irritation.

**Symptoms/injuries after ingestion**: No information available.

### SECTION 5: Firefighting measures

#### 5.1. Extinguishing media


**Unsuitable extinguishing media**: Do not use straight streams.

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

**Fire hazard**: Irritating fumes and organic acid vapors may develop when material is exposed to elevated temperatures or open flame.

#### 5.3. Advice for firefighters

**Firefighting instructions**: Exercise caution when fighting any chemical fire. Use water spray or fog for cooling exposed containers.

**Protection during firefighting**: Do not enter fire area without proper protective equipment, including respiratory protection. Avoid contact with skin and eyes. Do not breathe dust.

### SECTION 6: Accidental release measures

#### 6.1. Personal precautions, protective equipment and emergency procedures

##### 6.1.1. For non-emergency personnel

**Protective equipment**: Wear protective equipment as described in Section 8.

**Emergency procedures**: Evacuate unnecessary personnel.

##### 6.1.2. For emergency responders

**Protective equipment**: Do not attempt to take action without suitable protective equipment. Equip cleanup crew with proper protection. For further information refer to section 8: "Exposure controls/personal protection".

#### 6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if product enters sewers or public waters.

#### 6.3. Methods and material for containment and cleaning up

**For containment**: Contain any spills with dikes or absorbents to prevent migration and entry into sewers or streams.

**Methods for cleaning up**: Sweep or shovel spills into appropriate container for disposal.

#### 6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.
### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

- **Precautions for safe handling**: Avoid contact with skin and eyes. Do not breathe dust. Avoid dust formation. Provide local exhaust or general room ventilation to minimize exposure to dust.

- **Hygiene measures**: Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.

#### 7.2. Conditions for safe storage, including any incompatibilities

- **Storage conditions**: Keep container tightly closed.

- **Incompatible materials**: Oxidizing agent.

- **Storage area**: Store in a well-ventilated place. Store away from heat.

#### 7.3. Specific end use(s)

No additional information available

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

No additional information available

#### 8.2. Exposure controls

- **Appropriate engineering controls**: Provide local exhaust or general room ventilation.

- **Personal protective equipment**: Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

- **Hand protection**: Neoprene or nitrile rubber gloves.

- **Eye protection**: Chemical goggles. Contact lenses should not be worn.

- **Skin and body protection**: Wear suitable protective clothing.

- **Respiratory protection**: Where exposure through inhalation may occur from use, respiratory protection equipment is recommended. NIOSH-certified dust and mist (teal cartridge) respirator.

### SECTION 9: Physical and chemical properties

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

- **Physical state**: Solid

- **Appearance**: Solid.

- **Molecular mass**: 575.94 g/mol

- **Color**: Off-white.

- **Odor**: No data available

- **Odor threshold**: No data available

- **Refractive index**: No data available

- **pH**: No data available

- **Relative evaporation rate (butyl acetate=1)**: No data available

- **Melting point**: 110 °C

- **Freezing point**: No data available

- **Boiling point**: 140 °C @ 0.1 mm Hg

- **Flash point**: > 110 °C

- **Auto-ignition temperature**: No data available

- ** Decomposition temperature**: No data available

- **Flammability (solid, gas)**: No data available

- **Vapor pressure**: No data available

- **Relative vapor density at 20 °C**: No data available

- **Relative density**: No data available

- **VOC content**: > 5 %

- **Solubility**: Insoluble in water. Reacts with water.

- **Log Pow**: No data available

- **Log Kow**: No data available

- **Viscosity, kinematic**: No data available

- **Viscosity, dynamic**: No data available

- **Explosive properties**: No data available

- **Oxidizing properties**: No data available
Explosion limits : No data available

9.2. Other information
No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity
No additional information available

10.2. Chemical stability
Stable.

10.3. Possibility of hazardous reactions
Material decomposes slowly in contact with moist air or with water liberating isopropanol.

10.4. Conditions to avoid
Heat. Open flame. Sparks.

10.5. Incompatible materials
Oxidizing agent.

10.6. Hazardous decomposition products

SECTION 11: Toxicological information

11.1. Information on toxicological effects
Acute toxicity : Not classified
Skin corrosion/irritation : Not classified
Serious eye damage/irritation : Causes serious eye irritation.
Respiratory or skin sensitization : Not classified
Germ cell mutagenicity : Not classified
Carcinogenicity : Not classified
Reproductive toxicity : Not classified
Specific target organ toxicity (single exposure) : Not classified
Specific target organ toxicity (repeated exposure) : Not classified
Aspiration hazard : Not classified
Potential Adverse human health effects and symptoms : This compound liberates isopropanol on contact with moisture. Material generates isopropanol on contact with water or moisture in skin, eyes and mucous membranes and has an irritating, dehydrating effect on overexposed tissue.
Symptoms/injuries after inhalation : May cause irritation to the respiratory tract.
Symptoms/injuries after skin contact : May cause skin irritation.
Symptoms/injuries after eye contact : Causes serious eye irritation.
Symptoms/injuries after ingestion : No information available.
Reason for classification : Expert judgment

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
Effect on ozone layer : No additional information available
Effect on the global warming : No known ecological damage caused by this product.
SECTION 13: Disposal considerations

13.1. Waste treatment methods
Sewage disposal recommendations: Do not dispose of waste into sewer.
Waste disposal recommendations: Incinerate. Dispose in a safe manner in accordance with local/national regulations. Dispose of solid materials or residues at a licensed site.
Ecology - waste materials: Avoid release to the environment.

SECTION 14: Transport information

14.1. UN number
Not regulated for transport.

14.2. UN proper shipping name
Not applicable

14.3. Additional information
Other information: No supplementary information available.

Transport by sea
No additional information available

Air transport
No additional information available

SECTION 15: Regulatory information

15.1. US Federal regulations

ZIRCONIUM DIISOPROPOXIDE BIS(2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONATE), tech-90 (204522-78-1)

TSCA Exemption/Exclusion
CAUTION: This material is supplied for research and development purposes subject to the R&D exemption under TSCA, 40 CFR 720.36, and must meet the requirements of the exemption, including supervision by a "technically qualified individual" as defined by 40 CFR 720.3(ee). The use of this material for "commercial purposes" as defined by 40 CFR 720.3(r) is not permitted in the United States.

Zirconiunm diisopropoxide bis(2,2,6,6-tetramethyl-3,5-heptanedionate) (204522-78-1)
Not listed on the United States TSCA (Toxic Substances Control Act) inventory

15.2. International regulations
No additional information available

15.3. US State regulations

ZIRCONIUM DIISOPROPOXIDE BIS(2,2,6,6-TETRAMETHYL-3,5-HEPTANEDIONATE), tech-90(204522-78-1)

<table>
<thead>
<tr>
<th>State</th>
<th>Carcinogens List</th>
<th>Developmental Toxicity - Female</th>
<th>Developmental Toxicity - Male</th>
<th>Reproductive Toxicity - Female</th>
<th>Reproductive Toxicity - Male</th>
</tr>
</thead>
<tbody>
<tr>
<td>U.S.</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>U.S.</td>
<td>California - Proposition 65</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
<tr>
<td>U.S.</td>
<td>California - Proposition 65</td>
<td>No</td>
<td>No</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

Zirconium diisopropoxide bis(2,2,6,6-tetramethyl-3,5-heptanedionate) (204522-78-1)

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</tr>
<tr>
<td>U.S.</td>
<td>California - Proposition 65</td>
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<td>No</td>
<td>No</td>
<td>No</td>
</tr>
</tbody>
</table>

SECTION 16: Other information

Abbreviations and acronyms:
Abbreviations: ND: Not Determined, No Data; NA: Not Applicable; LD: Lethal Dose; LC: Lethal Concentration; ATE: Acute Toxicity Estimates; H: hour; °: °C unless otherwise stated; mm: millimeters Hg, torr; PEL: permissible exposure level; TWA: time weighted average; TLV: threshold limit value; TG: Test Guideline; NIOSH: National Institute for Occupational Safety and Health; IARC: International Agency for Research on Cancer; NTP: National Toxicology Program; HMIS: Hazardous Material Information System; CAS No.: Chemical Abstract Service Registration Number; EC No.: European Commission Registration Number; EC Index No.: European Commission Index Number; OECD: The Organisation for Economic Co-operation and Development.
Full text of H-phrases:

<table>
<thead>
<tr>
<th>Eye Irrit. 2A</th>
<th>Serious eye damage/eye irritation Category 2A</th>
</tr>
</thead>
<tbody>
<tr>
<td>H319</td>
<td>Causes serious eye irritation</td>
</tr>
</tbody>
</table>

HMIS III Rating

<table>
<thead>
<tr>
<th>Health</th>
<th>2 Moderate Hazard - Temporary or minor injury may occur</th>
</tr>
</thead>
<tbody>
<tr>
<td>Flammability</td>
<td>1 Slight Hazard</td>
</tr>
<tr>
<td>Physical</td>
<td>1 Slight Hazard</td>
</tr>
</tbody>
</table>

Prepared by safety and environmental affairs.

Date of issue: 10/19/2015       Version: 1.0

SDS US (GHS HazCom 2012) - Custom

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

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