

# ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE), 95%

Safety Data Sheet AKZ941

Date of issue: 01/17/2017      Version: 1.0

## SECTION 1: Identification

### 1.1. Product identifier

Product name	: ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE), 95%
Product code	: AKZ941
Product form	: Substance
Physical state	: Liquid
Formula	: C60H123O15P3Zr
Synonyms	: (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIY)TRIS(DIOCTYLPHOSPHATO)ZIRCONATE
Chemical family	: METAL COMPOUND

### 1.2. Recommended use of the chemical and restrictions on use

Recommended use	: Chemical intermediate For research use only
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### 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](mailto:info@gelest.com) - [www.gelest.com](http://www.gelest.com)

### 1.4. Emergency telephone number

Emergency number	: CHEMTREC: 1-800-424-9300 (USA); +1 703-527-3887 (International)
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## SECTION 2: Hazard(s) identification

### 2.1. Classification of the substance or mixture

#### GHS-US classification

Flammable liquids Category 4	H227
Serious eye damage/eye irritation Category 2A	H319
Full text of H statements	: see section 16

### 2.2. Label elements

#### GHS-US labeling

Hazard pictograms (GHS-US)



GHS07

Signal word (GHS-US)

: Warning

Hazard statements (GHS-US)

: H227 - Combustible liquid  
H319 - Causes serious eye irritation

Precautionary statements (GHS-US)

: P280 - Wear protective gloves/protective clothing/eye protection/face protection  
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  
P210 - Keep away from heat, open flames, sparks. - No smoking  
P370+P378 - In case of fire: Use water spray, foam, carbon dioxide, dry chemical to extinguish  
P403+P235 - Keep in a cool place  
P501 - Dispose of contents/container to licensed waste disposal facility

### 2.3. Hazards not otherwise classified (HNOC)

No additional information available

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

No data available

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Substance type	: Mono-constituent
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# ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE), 95%

## Safety Data Sheet

Name : ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE), 95%  
CAS No : 111053-49-7

Name	Product identifier	%	GHS-US classification
Zirconium (bis-2-2-(allyloxymethyl)butoxide)tris(dioctylphosphate)	(CAS No) 111053-49-7	95 - 100	Flam. Liq. 4, H227 Eye Irrit. 2A, H319

Full text of hazard classes and H-statements : see section 16

### 3.2. Mixtures

Not applicable

### 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.

### 4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

## SECTION 5: Firefighting measures

### 5.1. Extinguishing media

- Suitable extinguishing media : Water spray. Foam. Carbon dioxide. Dry chemical.
- Unsuitable extinguishing media : Do not use straight streams.

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

- Fire hazard : Combustible liquid. 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 to cool exposed surfaces.
- Protection during firefighting : Do not enter fire area without proper protective equipment, including respiratory protection. Avoid all eye and skin contact and do not breathe vapor and mist.

## SECTION 6: Accidental release measures

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

- General measures : Remove ignition sources. Use special care to avoid static electric charges.

#### 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 liquid 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 : Clean up any spills as soon as possible, using an absorbent material to collect it. Use only non-sparking tools.

### 6.4. Reference to other sections

See Heading 8. Exposure controls and personal protection.

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### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

- Additional hazards when processed : Keep away from heat/sparks/open flames/hot surfaces. - No smoking.
- Precautions for safe handling : Avoid all eye and skin contact and do not breathe vapor and mist. Ground/bond container and receiving equipment. Provide good ventilation in process area to prevent accumulation of vapors. Use only non-sparking tools.
- Hygiene measures : Wash contaminated clothing before reuse. Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work.

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

- Storage conditions : Keep container tightly closed. Keep in a cool place.
- Incompatible materials : Water.
- Storage area : Store in a well-ventilated place. Store away from heat.

### SECTION 8: Exposure controls/personal protection

#### 8.1. Control parameters

Zirconium (bis-2-2-(allyloxymethyl)butoxide)tris(dioctylphosphate) (111053-49-7)		
ACGIH	ACGIH TWA (mg/m <sup>3</sup> )	5 mg/m <sup>3</sup> Zr

#### 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 organic vapor (black cartridge) respirator.

### SECTION 9: Physical and chemical properties

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

- Physical state : Liquid
- Appearance : Viscous liquid.
- Molecular mass : 1328.28 g/mol
- Color : Amber.
- Odor : Characteristic.
- 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 : < 0 °C
- Freezing point : No data available
- Boiling point : > 150 °C @ 1 mm Hg
- Flash point : 76 °C
- Auto-ignition temperature : No data available
- Decomposition temperature : No data available
- Flammability (solid, gas) : Combustible liquid
- Vapor pressure : No data available
- Relative vapor density at 20 °C : > 1
- Relative density : 1.06
- Solubility : Reacts with water.
- Log Pow : No data available
- Log Kow : No data available
- Viscosity, kinematic : 140 - 180 cSt
- Viscosity, dynamic : No data available
- Explosive properties : No data available

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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 water.

### 10.4. Conditions to avoid

Heat. Open flame. Sparks.

### 10.5. Incompatible materials

Water.

### 10.6. Hazardous decomposition products

Organic acid vapors. Zirconium oxide fumes.

## 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  
None of the components in this product at concentrations >0.1% are listed by IARC, NTP, OSHA or ACGIH as a carcinogen  
Reproductive toxicity : Not classified  
Specific target organ toxicity – single exposure : Not classified  
Specific target organ toxicity – repeated exposure : Not classified  
Aspiration hazard : Not classified  
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 effects from this product.

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GWPmix comment : No known effects from this product.

### SECTION 13: Disposal considerations

#### 13.1. Waste treatment methods

Sewage disposal recommendations : Do not dispose of waste into sewer.  
Waste disposal recommendations : Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.  
Ecology - waste materials : Avoid release to the environment.

### SECTION 14: Transport information

#### 14.1. UN number

DOT NA no. NA1993

#### 14.2. UN proper shipping name

Transport document description : NA1993 Combustible liquid, n.o.s. (ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE)), 3, III  
Proper Shipping Name (DOT) : Combustible liquid, n.o.s.  
(ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE))  
Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120  
Packing group (DOT) : III - Minor Danger  
DOT Packaging Non Bulk (49 CFR 173.xxx) : 203  
DOT Packaging Bulk (49 CFR 173.xxx) : 241  
DOT Packaging Exceptions (49 CFR 173.xxx) : 150  
DOT Symbols : D - Proper shipping name for domestic use only, or to and from Canada, G - Identifies PSN requiring a technical name

#### 14.3. Additional information

Other information : No supplementary information available.  
Special transport precautions : This product is Combustible as defined by the US Department of Transportation (DOT). It is regulated for transport in the US in container > 119 gallons or 450 liters. The product is not regulated for transport by the IATA, ADR/RID, ADNR or the IMDG regulations.

#### Transport by sea

DOT Vessel Stowage Location : A - The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel

#### Air transport

DOT Quantity Limitations Passenger aircraft/rail : 60 L  
(49 CFR 173.27)  
DOT Quantity Limitations Cargo aircraft only (49 : 220 L  
CFR 175.75)

### SECTION 15: Regulatory information

#### 15.1. US Federal regulations

##### ZIRCONIUM (BIS-2-2-(ALLYLOXYMETHYL)BUTOXIDE)TRIS(DIOCTYLPHOSPHATE), 95% (111053-49-7)

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

##### Zirconium (bis-2-2-(allyloxymethyl)butoxide)tris(dioctylphosphate) (111053-49-7)

Not listed on the United States TSCA (Toxic Substances Control Act) inventory

#### 15.2. International regulations

##### CANADA

No additional information available

##### EU-Regulations

No additional information available

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### National regulations

No additional information available

### 15.3. US State regulations

No additional information available

## SECTION 16: Other information

Full text of H-phrases::

H227	Combustible liquid
H319	Causes serious eye irritation

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; GHS: The Globally Harmonized System of Classification and Labelling.

### 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 : 1 Slight Hazard - Materials that are normally stable but can become unstable (self-react) at high temperatures and pressures. Materials may react non-violently with water or undergo hazardous polymerization in the absence of inhibitors.

Prepared by safety and environmental affairs.

Date of issue: 01/17/2017 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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