



# ZIRCONIUM BIS(DIETHYLCITRATO)DI-n-PROPOXIDE, 75% in n-propanol/ethanol

Safety Data Sheet AKZ938.6

Date of issue: 10/19/2016 Version: 1.0

## SECTION 1: Identification

### 1.1. Identification

Product name	: ZIRCONIUM BIS(DIETHYLCITRATO)DI-n-PROPOXIDE, 75% in n-propanol/ethanol
Product code	: AKZ938.6
Product form	: Mixture
Physical state	: Liquid
Formula	: C <sub>26</sub> H <sub>44</sub> O <sub>16</sub> Zr
Synonyms	: ZIRCONIUM ETHYLCITRATE BIS[1,3-DIETHYL 2-(HYDROXY-KO)-1,2,3-PROPANETRICARBOXYLATO-KO <sub>2</sub> ]DIPROPOXYZIRCONIUM ZIRCONIUM, BIS[1,3-DIETHYL 2-(HYDROXY-KO)-1,2,3-PROPANETRICARBOXYLATO-KO <sub>2</sub> ]DIPROPOXY-
Chemical family	: METAL ALKOXIDE

### 1.2. Recommended use and restrictions on use

Recommended use	: Chemical intermediate
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### 1.3. Supplier

#### 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 2	H225 Highly flammable liquid and vapor
Skin corrosion/irritation Category 2	H315 Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319 Causes serious eye irritation
Specific target organ toxicity (single exposure) Category 3	H336 May cause drowsiness or dizziness

Full text of H statements : see section 16

### 2.2. GHS Label elements, including precautionary statements

#### GHS US labeling

Hazard pictograms (GHS US)	:	
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Signal word (GHS US)	: Danger
Hazard statements (GHS US)	: H225 - Highly flammable liquid and vapor H315 - Causes skin irritation H319 - Causes serious eye irritation H336 - May cause drowsiness or dizziness
Precautionary statements (GHS US)	: P280 - Wear protective gloves/protective clothing/eye protection/face protection. P312 - Call a doctor if you feel unwell P210 - Keep away from heat, open flames, sparks. - No smoking. P240 - Ground/Bond container and receiving equipment P241 - Use explosion-proof electrical equipment P242 - Use only non-sparking tools. P243 - Take precautionary measures against static discharge. P261 - Avoid breathing vapors. P264 - Wash hands thoroughly after handling. P271 - Use only outdoors or in a well-ventilated area. P303+P361+P353 - If on skin (or hair): take off immediately all contaminated clothing. rinse skin with water/shower P332+P313 - If skin irritation occurs: Get medical advice/attention. P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove

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contact lenses, if present and easy to do. Continue rinsing  
P337+P313 - If eye irritation persists: Get medical advice/attention.  
P321 - Specific treatment (see first aid instructions on this label)  
P362+P364 - Take off contaminated clothing and wash it before reuse.  
P370+P378 - In case of fire: Use water spray, foam, carbon dioxide, dry chemical to extinguish.  
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.  
P403+P235 - Keep in a cool place  
P405 - Store locked up.  
P501 - Dispose of contents/container to licensed waste disposal facility.

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

Other hazards not contributing to the classification : Material may form zirconium oxides or zirconate polymers on the skin, eyes or in the lungs. Prolonged exposure to zirconium compounds can induce formation of granulomatous lesions in the lungs or on the skin.

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

Not applicable

## SECTION 3: Composition/Information on ingredients

### 3.1. Substances

Not applicable

### 3.2. Mixtures

Name	Product identifier	%	GHS-US classification
Zirconium bis(diethylcitrate)di-n-propoxide	(CAS-No.) 308847-92-9	75	Eye Irrit. 2A, H319
n-Propanol	(CAS-No.) 71-23-8	10 - 25	Flam. Liq. 3, H226 Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H336
Ethanol	(CAS-No.) 64-17-5	5 - 10	Flam. Liq. 2, H225 Eye Irrit. 2A, H319

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

## 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 (acute and delayed)

Symptoms/effects after inhalation : May cause drowsiness or dizziness. May cause irritation to the respiratory tract.

Symptoms/effects after skin contact : Causes skin irritation.

Symptoms/effects after eye contact : Causes serious eye irritation.

Symptoms/effects after ingestion : May be harmful if swallowed.

### 4.3. Immediate medical attention and special treatment, if necessary

No additional information available

## SECTION 5: Fire-fighting measures

### 5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media : Water spray. Foam. Carbon dioxide. Dry chemical.

Unsuitable extinguishing media : Do not use straight streams.

### 5.2. Specific hazards arising from the chemical

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

Explosion hazard : May form flammable/explosive vapor-air mixture.

### 5.3. Special protective equipment and precautions for fire-fighters

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.

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### SECTION 6: Accidental release measures

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

General measures : Eliminate every possible source of ignition. 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.

### SECTION 7: Handling and storage

#### 7.1. Precautions for safe handling

Additional hazards when processed : Handle empty containers with care because residual vapors are flammable. 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. Take precautionary measures against static discharge. 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

Technical measures : Proper grounding procedures to avoid static electricity should be followed. Use explosion-proof electrical equipment.

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

n-Propanol (71-23-8)		
ACGIH	ACGIH TWA (ppm)	100 ppm
OSHA	OSHA PEL (TWA) (mg/m <sup>3</sup> )	500 mg/m <sup>3</sup>
OSHA	OSHA PEL (TWA) (ppm)	200 ppm
IDLH	US IDLH (ppm)	800 ppm
NIOSH	NIOSH REL (TWA) (mg/m <sup>3</sup> )	500 mg/m <sup>3</sup>
NIOSH	NIOSH REL (TWA) (ppm)	200 ppm
NIOSH	NIOSH REL (STEL) (mg/m <sup>3</sup> )	625 mg/m <sup>3</sup>
NIOSH	NIOSH REL (STEL) (ppm)	250 ppm

Ethanol (64-17-5)		
ACGIH	ACGIH STEL (ppm)	1000 ppm
OSHA	OSHA PEL (TWA) (mg/m <sup>3</sup> )	1900 mg/m <sup>3</sup>
OSHA	OSHA PEL (TWA) (ppm)	1000 ppm
IDLH	US IDLH (ppm)	3300 ppm (10% LEL)
NIOSH	NIOSH REL (TWA) (mg/m <sup>3</sup> )	1900 mg/m <sup>3</sup>

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### Ethanol (64-17-5)

NIOSH	NIOSH REL (TWA) (ppm)	1000 ppm
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### 8.2. Appropriate engineering controls

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

### 8.3. Individual protection measures/Personal protective equipment

#### 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	: 703.84 g/mol
Color	: Colorless.
Odor	: No data available
Odor threshold	: No data available
Refractive index	: 1.451
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Melting point	: No data available
Freezing point	: No data available
Boiling point	: 97 °C - initial (n-propanol)
Flash point	: 14 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Highly flammable liquid and vapor
Vapor pressure	: ~ 20 mm Hg @ 25°C
Relative vapor density at 20 °C	: 2.1 (n-propanol)
Relative density	: 1.14
% Volatiles	: > 30 %
Solubility	: 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	: 2.2 - 13.7 vol % (lower; upper; n-propanol)

### 9.2. Other information

No additional information available

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### 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

<b>n-Propanol (71-23-8)</b>	
LD50 oral rat	1870 mg/kg
LD50 dermal rabbit	4049 mg/kg
LC50 inhalation rat (ppm)	> 13548 ppm/4h

<b>Zirconium bis(diethylcitrate)di-n-propoxide (308847-92-9)</b>	
LD50 oral rat	> 3000 mg/kg

<b>Ethanol (64-17-5)</b>	
LD50 oral rat	7060 mg/kg
LC50 inhalation rat (mg/l)	124.7 mg/l/4h
LC50 inhalation rat (ppm)	20000 ppm 10 hrs.
LDLo oral rat	1400 mg/kg (Human)
ATE US (oral)	7060 mg/kg body weight
ATE US (vapors)	124.7 mg/l/4h
ATE US (dust, mist)	124.7 mg/l/4h

Skin corrosion/irritation : Causes skin irritation.

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.

<b>Ethanol (64-17-5)</b>	
IARC group	1 - Carcinogenic to humans
In OSHA Hazard Communication Carcinogen list	Yes

Reproductive toxicity : Not classified

Specific target organ toxicity – single exposure : May cause drowsiness or dizziness.

Specific target organ toxicity – repeated exposure : Not classified

Aspiration hazard : Not classified

Symptoms/effects after inhalation : May cause drowsiness or dizziness. May cause irritation to the respiratory tract.

Symptoms/effects after skin contact : Causes skin irritation.

Symptoms/effects after eye contact : Causes serious eye irritation.

Symptoms/effects after ingestion : May be harmful if swallowed.

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### SECTION 12: Ecological information

#### 12.1. Toxicity

n-Propanol (71-23-8)	
LC50 fish 1	4480 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
EC50 Daphnia 1	3642 mg/l (Exposure time: 48 h - Species: Daphnia magna)
EC50 Daphnia 2	3339 - 3977 mg/l (Exposure time: 48 h - Species: Daphnia magna [Static])
Ethanol (64-17-5)	
LC50 fish 1	> 10000 mg/l (Exposure time: 96 h - Species: Oncorhynchus mykiss [static])
LC50 fish 2	> 13400 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])

#### 12.2. Persistence and degradability

No additional information available

#### 12.3. Bioaccumulative potential

n-Propanol (71-23-8)	
Log Pow	0.25 - 0.34
Ethanol (64-17-5)	
Log Pow	-0.32

#### 12.4. Mobility in soil

No additional information available

#### 12.5. Other adverse effects

Other adverse effects : This substance may be hazardous to the environment.  
Effect on the ozone layer : No additional information available

### SECTION 13: Disposal considerations

#### 13.1. Disposal methods

Sewage disposal recommendations : Do not dispose of waste into sewer.  
Product/Packaging disposal recommendations : Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.  
Additional information : Handle empty containers with care because residual vapors are flammable.  
Ecology - waste materials : Avoid release to the environment.

### SECTION 14: Transport information

#### 14.1. UN number

UN-No.(DOT) : 1993  
DOT NA no. : UN1993

#### 14.2. UN proper shipping name

Transport document description : UN1993 Flammable liquids, n.o.s. (ZIRCONIUM BIS(DIETHYLCITRATO)DI-n-PROPOXIDE, 75% in n-propanol/ethanol), 3, II  
Proper Shipping Name (DOT) : Flammable liquids, n.o.s.  
(ZIRCONIUM BIS(DIETHYLCITRATO)DI-n-PROPOXIDE, 75% in n-propanol/ethanol)  
Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120  
Packing group (DOT) : II - Medium Danger  
Hazard labels (DOT) : 3 - Flammable liquid



DOT Packaging Non Bulk (49 CFR 173.xxx) : 202  
DOT Packaging Bulk (49 CFR 173.xxx) : 242  
DOT Packaging Exceptions (49 CFR 173.xxx) : 150  
DOT Symbols : G - Identifies PSN requiring a technical name

#### 14.3. Additional information

Emergency Response Guide (ERG) Number : 128  
Other information : No supplementary information available.

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### Transport by sea

DOT Vessel Stowage Location : B - (i) The material may be stowed "on deck" or "under deck" on a cargo vessel and on a passenger vessel carrying a number of passengers limited to not more than the larger of 25 passengers, or one passenger per each 3 m of overall vessel length; and (ii) "On deck only" on passenger vessels in which the number of passengers specified in paragraph (k)(2)(i) of this section is exceeded.

### Air transport

DOT Quantity Limitations Passenger aircraft/rail : 5 L  
(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 60 L  
CFR 175.75)

## SECTION 15: Regulatory information

### 15.1. US Federal regulations

#### ZIRCONIUM BIS(DIETHYLCITRATO)DI-n-PROPOXIDE, 75% in n-propanol/ethanol (308847-92-9)

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.

#### n-Propanol (71-23-8)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

#### Zirconium bis(diethylcitrate)di-n-propoxide (308847-92-9)

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

#### Ethanol (64-17-5)

Listed on the United States TSCA (Toxic Substances Control Act) inventory

### 15.2. International regulations

#### CANADA

##### n-Propanol (71-23-8)

Listed on the Canadian DSL (Domestic Substances List)

WHMIS Classification

Class B Division 2 - Flammable Liquid  
Class D Division 2 Subdivision B - Toxic material causing other toxic effects

##### Ethanol (64-17-5)

Listed on the Canadian DSL (Domestic Substances List)

WHMIS Classification

Class B Division 2 - Flammable Liquid  
Class D Division 2 Subdivision B - Toxic material causing other toxic effects

### EU-Regulations

#### n-Propanol (71-23-8)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

#### Ethanol (64-17-5)

Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)

### National regulations

#### n-Propanol (71-23-8)

Listed on the AICS (Australian Inventory of Chemical Substances)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory  
Listed on the Korean ECL (Existing Chemicals List)  
Listed on NZIoC (New Zealand Inventory of Chemicals)  
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)  
Listed on the Canadian IDL (Ingredient Disclosure List)  
Listed on INSQ (Mexican National Inventory of Chemical Substances)  
Listed on CICR (Turkish Inventory and Control of Chemicals)

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### Ethanol (64-17-5)

Listed on IARC (International Agency for Research on Cancer)  
Listed on the AICS (Australian Inventory of Chemical Substances)  
Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)  
Listed on the Japanese ENCS (Existing & New Chemical Substances) inventory  
Listed on the Korean ECL (Existing Chemicals List)  
Listed on NZIoC (New Zealand Inventory of Chemicals)  
Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)  
Listed on the Canadian IDL (Ingredient Disclosure List)  
Listed on INSQ (Mexican National Inventory of Chemical Substances)  
Listed on CICR (Turkish Inventory and Control of Chemicals)

### 15.3. US State regulations

**WARNING:** This product can expose you to Ethanol, which is known to the State of California to cause cancer and birth defects or other reproductive harm. For more information go to [www.P65Warnings.ca.gov](http://www.P65Warnings.ca.gov).

### Ethanol (64-17-5)

U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No significant risk level (NSRL)	Maximum allowable dose level (MADL)
Yes	Yes	No	No		

### n-Propanol (71-23-8)

U.S. - Massachusetts - Right To Know List  
U.S. - New Jersey - Right to Know Hazardous Substance List  
U.S. - Pennsylvania - RTK (Right to Know) List

### Ethanol (64-17-5)

U.S. - Massachusetts - Right To Know List  
U.S. - New Jersey - Right to Know Hazardous Substance List  
U.S. - Pennsylvania - RTK (Right to Know) List

## SECTION 16: Other information

Full text of H-phrases::

H225	Highly flammable liquid and vapor
H226	Flammable liquid and vapor
H302	Harmful if swallowed
H315	Causes skin irritation
H319	Causes serious eye irritation
H336	May cause drowsiness or dizziness

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; APF: Assigned Protection Factor.

### Hazard Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur  
Flammability : 3 Serious Hazard - Materials capable of ignition under almost all normal temperature conditions. Includes flammable liquids with flash points below 73 F and boiling points above 100 F. as well as liquids with flash points between 73 F and 100 F. (Classes IB & IC)  
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: 10/19/2016 Version: 1.0



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SDS US (GHS HazCom 2012) - Custom

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

*The information contained in this document has been gathered from reference materials and/or Gelest, Inc. test data and is to the best knowledge and belief of Gelest, Inc. accurate and reliable. Such information is offered solely for your consideration, investigation and verification. It is not suggested or guaranteed that the hazard precautions or procedures described are the only ones which exist. Gelest, Inc. makes no warranties, express or implied, with respect to the use of such information and assumes no responsibility therefore. Information on this safety data sheet is not intended to constitute a basis for product specifications.*

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