

Safety Data Sheet AKT851.3
Date of issue: 11/28/2016 Version: 1.4

SECTION 1: Identification

1.1. Identification

Product name : TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M in heptane

Product code : AKT851.3
Product form : Mixture
Physical state : Liquid
Formula : C9H21CIO3Ti

Synonyms : TRIISOPROPYLCHLOROTITANATE

CHLOROTITANIUM TRIISOPROPOXIDE

Chemical family : METAL ESTER

1.2. Recommended use and restrictions on use

Recommended use : Chemical intermediate

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 - www.gelest.com

1.4. Emergency telephone number

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

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Flammable liquids Category 2

Skin corrosion/irritation Category 1B

Full text of H statements: see section 16

Serious eye damage/eye irritation Category 1

Specific target organ toxicity (single exposure) Category 3

Hazardous to the aquatic environment - Acute Hazard Category 1

Hazardous to the aquatic environment - Chronic Hazard Category 1

H225 Highly flammable liquid and vapor

H314 Causes severe skin burns and eye damage

H318 Causes serious eye damage H336 May cause drowsiness or dizziness

H400 Very toxic to aquatic life

H410 Very toxic to aquatic life with long lasting effects

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US)









Signal word (GHS US) : Danger

Hazard statements (GHS US) : H225 - Highly flammable liquid and vapor

H314 - Causes severe skin burns and eye damage

H318 - Causes serious eye damage
H336 - May cause drowsiness or dizziness

H400 - Very toxic to aquatic life

H410 - Very toxic to aquatic life with long lasting effects

Precautionary statements (GHS US) : P280 - Wear protective gloves/protective clothing/eye protection/face protection.

P310 - Immediately call a doctor

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.

P260 - Do not breathe vapors.

P264 - Wash hands thoroughly after handling. P271 - Use only outdoors or in a well-ventilated area.

P273 - Avoid release to the environment.

P301+P330+P331 - If swallowed: rinse mouth. Do NOT induce vomiting

P303+P361+P353 - If on skin (or hair): take off immediately all contaminated clothing. rinse

skin with water/shower

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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

contact lenses, if present and easy to do. Continue rinsing

P312 - Call a doctor if you feel unwell

P321 - Specific treatment (see first aid instructions on this label)

P363 - Wash contaminated clothing before reuse.

P370+P378 - In case of fire: Use water spray or fog, foam, carbon dioxide, dry chemical to extinguish.

P391 - Collect spillage.

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)

No additional information available

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
Titanium chloride triisopropoxide	(CAS-No.) 20717-86-6	56 - 60	Flam. Sol. 2, H228 Skin Corr. 1B, H314 Eye Dam. 1, H318
n-Heptane	(CAS-No.) 142-82-5	40 - 44	Flam. Liq. 2, H225 Skin Irrit. 2, H315 STOT SE 3, H336 Asp. Tox. 1, H304 Aquatic Acute 1, H400 Aquatic Chronic 1, H410
Isopropanol	(CAS-No.) 67-63-0	0 - 2	Flam. Liq. 2, H225 Acute Tox. 4 (Oral), H302 Eye Irrit. 2A, H319 STOT SE 3, H336

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 immediate 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 immediate 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 : Causes severe skin burns and eye damage.

Symptoms/effects after inhalation : May cause drowsiness or dizziness. May cause irritation to the respiratory tract. Exposure at high levels may have narcotic effects. Heptane can cause vertigo, incoordination and stupor at

5000ppm. Vapor inhalation of heptane may lead to impairment of coordination mental

alertness, and reaction times, leading to accident proneness.

Symptoms/effects after skin contact : Causes (severe) skin burns.

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

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

4.3. Immediate medical attention and special treatment, if necessary

Note to physician: Activated charcoal slurry may be administered. Activated charcoal slurry is prepared by suspending 50 grams of activated charcoal in 400 ml water and mixing thoroughly. Administer 5 ml/kg.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

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

Unsuitable extinguishing media : Do not use straight streams.

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5.2. Specific hazards arising from the chemical

Fire hazard : Highly flammable liquid and vapor. Irritating fumes and caustic 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 or fog for cooling exposed

containers.

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 : 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

Avoid release to the environment. 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. Collect spillage.

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. Take precautionary measures against static discharge. Use only outdoors

or in a well-ventilated area. 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. Store locked up.

Incompatible materials : Oxidizing agent.

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

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Isopropanol (67-63-0)		
ACGIH	ACGIH TWA (ppm)	200 ppm
ACGIH	ACGIH STEL (ppm)	400 ppm
OSHA	OSHA PEL (TWA) (mg/m³)	980 mg/m³
OSHA	OSHA PEL (TWA) (ppm)	400 ppm
IDLH	US IDLH (ppm)	2000 ppm (10% LEL)
NIOSH	NIOSH REL (TWA) (mg/m³)	980 mg/m³
NIOSH	NIOSH REL (TWA) (ppm)	400 ppm
NIOSH	NIOSH REL (STEL) (mg/m³)	1225 mg/m³

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Isopropanol (67-63-0)		
NIOSH	NIOSH REL (STEL) (ppm)	500 ppm
n-Heptane (142-82-5)		
ACGIH	ACGIH TWA (ppm)	400 ppm
ACGIH	ACGIH STEL (ppm)	500 ppm
OSHA	OSHA PEL (TWA) (mg/m³)	2000 mg/m³
OSHA	OSHA PEL (TWA) (ppm)	500 ppm
IDLH	US IDLH (ppm)	750 ppm
NIOSH	NIOSH REL (TWA) (mg/m³)	350 mg/m³
NIOSH	NIOSH REL (TWA) (ppm)	85 ppm
NIOSH	NIOSH REL (ceiling) (mg/m³)	1800 mg/m³
NIOSH	NIOSH REL (ceiling) (ppm)	440 ppm

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 or face shield. 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

: Liquid Physical state Appearance : Liquid. : 260.62 g/mol Molecular mass : Pale yellow. Color Odor : No data available : No data available Odor threshold Refractive index : No data available рΗ : No data available Relative evaporation rate (butyl acetate=1) : No data available

Melting point : < 15 °C

Freezing point : No data available
Boiling point : 98 °C (initial, heptane)

Flash point : $-4 \, ^{\circ}\text{C}$ Auto-ignition temperature : $225 \, ^{\circ}\text{C}$

Decomposition temperature : No data available

Flammability (solid, gas) : Highly flammable liquid and vapor

Vapor pressure : No data available Relative vapor density at 20 °C : 2.97 (heptane)

Relative density : 0.91 % Volatiles : > 70 %

Solubility : Reacts with water.

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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 : 1.25 - 6.9 vol % (lower; upper: heptane)

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 and rapidly in contact with water liberating isopropanol.

10.4. Conditions to avoid

Heat. Sparks. Open flame.

10.5. Incompatible materials

Oxidizing agent.

10.6. Hazardous decomposition products

Hydrogen chloride. Isopropanol. Organic acid vapors. Titanium oxide.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Isopropanol (67-63-0)	
LD50 oral rat	1870 mg/kg
LD50 dermal rabbit	4059 mg/kg
LC50 inhalation rat (mg/l)	72600 mg/m³ (Exposure time: 4 h)
ATE US (oral)	1870 mg/kg body weight
ATE US (dermal)	4059 mg/kg body weight
n-Heptane (142-82-5)	
LD50 oral mouse	5000 mg/kg
LD50 dermal rabbit	3000 mg/kg
LC50 inhalation rat (mg/l)	103 g/m³ (Exposure time: 4 h)
ATE US (dermal)	3000 mg/kg body weight
ATE US (vapors)	103 mg/l/4h

1000 ppm Inhalation (heptane)-human, TCLo

Skin corrosion/irritation : Causes severe skin burns and eye damage.

Serious eye damage/irritation : Causes serious eye damage.

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.

Isopropanol (67-63-0)

ATE US (dust, mist)

Toxicity information

IARC group 3 - Not classifiable

Reproductive toxicity : Not classified

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

Specific target organ toxicity - repeated

exposure

: Not classified

103 mg/l/4h

Aspiration hazard : Not classified

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Potential Adverse human health effects and

symptoms

Symptoms/effects after inhalation

Material generates isopropanol on contact with water or moisture in skin, eyes and mucous

membranes and has an irritating, dehydrating effect on overexposed tissue.

May cause drowsiness or dizziness. May cause irritation to the respiratory tract. Exposure at high levels may have narcotic effects. Heptane can cause vertigo, incoordination and stupor at 5000ppm. Vapor inhalation of heptane may lead to impairment of coordination mental

alertness, and reaction times, leading to accident proneness.

Symptoms/effects after skin contact : Causes (severe) skin burns. Symptoms/effects after eye contact Causes serious eye damage. Symptoms/effects after ingestion : May be harmful if swallowed.

Reason for classification : Expert judgment

SECTION 12: Ecological information

Toxicity

: Very toxic to aquatic life. Very toxic to aquatic life with long lasting effects. Ecology - general

Isopropanol (67-63-0)		
LC50 fish 1	9640 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])	
EC50 Daphnia 1	13299 mg/l (Exposure time: 48 h - Species: Daphnia magna)	
LC50 fish 2	11130 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])	
n-Heptane (142-82-5)		
LC50 fish 1	375 mg/l (Exposure time: 96 h - Species: Cichlid fish)	

Persistence and degradability

No additional information available

12.3. **Bioaccumulative potential**

Isopropanol (67-63-0)		
Log Pow	0.05 (at 25 °C)	
n-Heptane (142-82-5)		
Log Pow	4.66	

12.4. Mobility in soil

No additional information available

Other adverse effects 12.5.

: No additional information available Effect on the ozone layer

SECTION 13: Disposal considerations

Disposal methods

Sewage disposal recommendations : Do not dispose of waste into sewer.

Dispose in a safe manner in accordance with local/national regulations. Dispose of Product/Packaging disposal recommendations

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) : 2924 DOT NA no. UN2924

UN proper shipping name

UN2924 Flammable liquids, corrosive, n.o.s. (TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M Transport document description

in heptane), 3 (8), II

Proper Shipping Name (DOT) : Flammable liquids, corrosive, n.o.s.

(TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M in heptane)

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 8 - Corrosive





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Dangerous for the environment Yes
Marine pollutant : Yes



DOT Packaging Non Bulk (49 CFR 173.xxx) : 202
DOT Packaging Bulk (49 CFR 173.xxx) : 243
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 : 132

Other information : No supplementary information available.

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.

DOT Vessel Stowage Other : 40 - Stow "clear of living quarters"

Air transport

DOT Quantity Limitations Passenger aircraft/rail : 1 L

(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 5 L

CFR 175.75)

SECTION 15: Regulatory information

15.1. US Federal regulations

Isopropanol (67-63-0)		
Listed on the United States TSCA (Toxic Subs Subject to reporting requirements of United Sta		
EPA TSCA Regulatory Flag	T - T - indicates a substance that is the subject of a final TSCA section 4 test rule.	
SARA Section 313 - Emission Reporting	1 % (only if manufactured by the strong acid process, no supplier notification)	
Titanium chloride triisopropoxide (20717-86	G-6)	
Listed on the United States TSCA (Toxic Subs	tances Control Act) inventory	
n-Heptane (142-82-5)		
Listed on the United States TSCA (Toxic Subs	tances Control Act) inventory	
EPA TSCA Regulatory Flag	A TSCA Regulatory Flag T - T - indicates a substance that is the subject of a final TSCA section 4 test rule.	

15.2. International regulations

CANADA

Isopropanol (67-63-0)		
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		
Titanium chloride triisopropoxide (20717-86-6)		
Listed on the Canadian NDSL (Non-Domestic Substances List)		
n-Heptane (142-82-5)		
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

Isopropanol (67-63-0)	
Listed on the EEC inventory EINECS (European Inventory of Existing Commercial Chemical Substances)	

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n-Heptane (142-82-5)

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

National regulations

Isopropanol (67-63-0)

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 Japanese ISHL (Industrial Safety and Health Law)

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)

Titanium chloride triisopropoxide (20717-86-6)

Listed on the AICS (Australian Inventory of Chemical Substances)

Listed on NZIoC (New Zealand Inventory of Chemicals)

Listed on PICCS (Philippines Inventory of Chemicals and Chemical Substances)

n-Heptane (142-82-5)

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

California Proposition 65 - This product does not contain any substances known to the state of California to cause cancer, developmental and/or reproductive harm

Isopropanol (67-63-0)

U.S. - Massachusetts - Right To Know List

U.S. - New Jersey - Right to Know Hazardous Substance List

U.S. - Pennsylvania - RTK (Right to Know) - Environmental Hazard List

U.S. - Pennsylvania - RTK (Right to Know) List

n-Heptane (142-82-5)

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::

ext of H-phrases::	
H225	Highly flammable liquid and vapor
H228	Flammable solid
H302	Harmful if swallowed
H304	May be fatal if swallowed and enters airways
H314	Causes severe skin burns and eye damage
H315	Causes skin irritation
H318	Causes serious eye damage
H319	Causes serious eye irritation
H336	May cause drowsiness or dizziness
H400	Very toxic to aquatic life
H410	Very toxic to aquatic life with long lasting effects

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.: Chemcial 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.

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Hazard Rating

Physical

Health : 3 Serious Hazard - Major injury likely unless prompt action is taken and medical treatment is

given

Flammability : 4 Severe Hazard - Flammable gases, or very volatile flammable liquids with flash points below

73 F, and boiling points below 100 F. Materials may ignite spontaneously with air. (Class IA)

: 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.

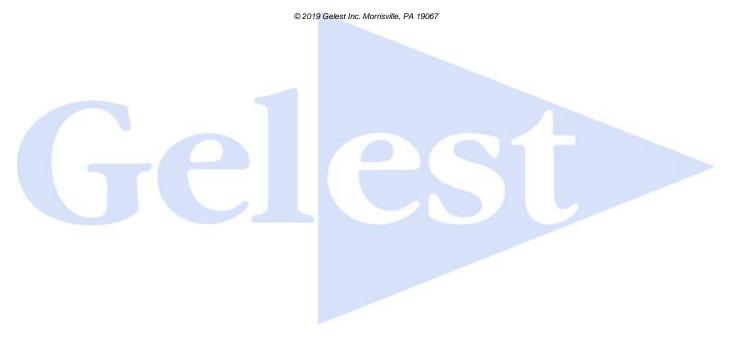
Prepared by safety and environmental affairs.

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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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