



TITANIUM CHLORIDE TRIISOPROPOXIDE, 1.25M in tetrahydrofuran

Safety Data Sheet AKT851.2

Date of issue: 03/15/2017

Version: 1.0

SECTION 1: Identification

1.1. Identification

Product name	: TITANIUM CHLORIDE TRIISOPROPOXIDE, 1.25M in tetrahydrofuran
Product code	: AKT851.2
Product form	: Mixture
Physical state	: Liquid
Formula	: C ₉ H ₂₁ ClO ₃ Ti
Synonyms	: TRIISOPROPYLCHLOROTITANATE CHLOROTITANIUM TRIISOPROPOXIDE
Chemical family	: METAL ESTER

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 - 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 1B	H314 Causes severe skin burns and eye damage
Serious eye damage/eye irritation Category 1	H318 Causes serious eye damage
Carcinogenicity Category 2	H351 Suspected of causing cancer
Specific target organ toxicity (single exposure) Category 3	H335 May cause respiratory irritation
Full text of H statements : see section 16	

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
H335 - May cause respiratory irritation
H351 - Suspected of causing cancer

Precautionary statements (GHS US) : P201 - Obtain special instructions before use.
P202 - Do not handle until all safety precautions have been read and understood.
P280 - Wear protective gloves/protective clothing/eye protection/face protection.
P308+P313 - If exposed or concerned: Get medical advice/attention.
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.
P261 - Avoid breathing vapors.
P264 - Wash hands thoroughly after handling.
P271 - Use only outdoors or in a well-ventilated area.
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
P310 - Immediately call a POISON CENTER
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.
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
Tetrahydrofuran	(CAS-No.) 109-99-9	65 - 70	Flam. Liq. 2, H225 Acute Tox. 4 (Oral), H302 Eye Irrit. 2A, H319 Carc. 2, H351 STOT SE 3, H335
Titanium chloride triisopropoxide	(CAS-No.) 20717-86-6	30 - 35	Flam. Sol. 2, H228 Skin Corr. 1B, H314 Eye Dam. 1, H318
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 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. Immediately call a poison center or doctor/physician.

4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects	: May cause cancer. Causes severe skin burns and eye damage.
Symptoms/effects after inhalation	: May cause respiratory irritation. Headache. Nausea.
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.
Chronic symptoms	: TETRAHYDROFURAN: Mildly toxic by inhalation. Mutagenic data has been reported. Reported as causing injury to liver and kidneys.

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 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 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".
- Emergency procedures : Ventilate area.

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. Sweep or shovel spills into appropriate container for disposal. 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 : Obtain special instructions before use. Do not handle until all safety precautions have been read and understood. 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

Tetrahydrofuran (109-99-9)		
ACGIH	ACGIH TWA (ppm)	50 ppm
ACGIH	ACGIH STEL (ppm)	100 ppm
OSHA	OSHA PEL (TWA) (mg/m ³)	590 mg/m ³
OSHA	OSHA PEL (TWA) (ppm)	200 ppm
IDLH	US IDLH (ppm)	2000 ppm (10% LEL)
NIOSH	NIOSH REL (TWA) (mg/m ³)	590 mg/m ³

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Tetrahydrofuran (109-99-9)		
NIOSH	NIOSH REL (TWA) (ppm)	200 ppm
NIOSH	NIOSH REL (STEL) (mg/m³)	735 mg/m³
NIOSH	NIOSH REL (STEL) (ppm)	250 ppm
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
NIOSH	NIOSH REL (STEL) (ppm)	500 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

Physical state	: Liquid
Appearance	: Liquid.
Molecular mass	: 260.62 g/mol
Color	: Pale yellow.
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	: < 15 °C
Freezing point	: No data available
Boiling point	: 66 °C -initial
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	: 114 mm Hg @ 15°C (THF)
Relative vapor density at 20 °C	: > 1

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Relative density	: 0.941
% Volatiles	: 25 %
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	: 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 and rapidly in contact with water liberating isopropanol.

10.4. Conditions to avoid

Heat. Open flame. Sparks.

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

Tetrahydrofuran (109-99-9)	
LD50 oral rat	1650 mg/kg
LC50 inhalation rat (ppm)	21000 ppm (Exposure time: 3 h)
ATE US (oral)	1650 mg/kg body weight
Isopropanol (67-63-0)	
LD50 oral rat	1870 mg/kg
LD50 dermal rabbit	4059 mg/kg
LC50 inhalation rat (mg/l)	72600 mg/m ³ (Exposure time: 4 h)
ATE US (oral)	1870 mg/kg body weight
ATE US (dermal)	4059 mg/kg body weight

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	: Suspected of causing cancer. This product contains a component that has been reported to be possibly carcinogenic based on its IARC, ACGIH classification.

Tetrahydrofuran (109-99-9)	
National Toxicology Program (NTP) Status	1 - Evidence of Carcinogenicity

Isopropanol (67-63-0)	
IARC group	3 - Not classifiable

Reproductive toxicity	: Not classified
Specific target organ toxicity – single exposure	: May cause respiratory irritation.

Specific target organ toxicity – repeated exposure	: Not classified
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Aspiration hazard	: Not classified
Potential Adverse human health effects and symptoms	: 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/effects after inhalation	: May cause respiratory irritation. Headache. Nausea.
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.
Chronic symptoms	: TETRAHYDROFURAN: Mildly toxic by inhalation. Mutagenic data has been reported. Reported as causing injury to liver and kidneys.
Reason for classification	: Expert judgment

SECTION 12: Ecological information

12.1. Toxicity

Ecology - water : Toxic to aquatic life. Toxic to aquatic life with long lasting effects.

Tetrahydrofuran (109-99-9)	
LC50 fish 1	1970 - 2360 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
LC50 fish 2	2700 - 3600 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])
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])

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Tetrahydrofuran (109-99-9)	
BCF fish 1	(will not bioconcentrate)
Log Pow	0.45 (at 25 °C)
Isopropanol (67-63-0)	
Log Pow	0.05 (at 25 °C)

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 : Incinerate. 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) : 2056
DOT NA no. UN2056

14.2. UN proper shipping name

Transport document description : UN2056 Tetrahydrofuran (TITANIUM CHLORIDE TRIISOPROPOXIDE, 1.25M in tetrahydrofuran), 3, II
Proper Shipping Name (DOT) : Tetrahydrofuran
(TITANIUM CHLORIDE TRIISOPROPOXIDE, 1.25M in tetrahydrofuran)
Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120
Packing group (DOT) : II - Medium Danger

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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) : None

14.3. Additional information

Emergency Response Guide (ERG) Number : 127

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.

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

Tetrahydrofuran (109-99-9)

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

EPA TSCA Regulatory Flag : T - T - indicates a substance that is the subject of a final TSCA section 4 test rule.

Titanium chloride triisopropoxide (20717-86-6)

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

Isopropanol (67-63-0)

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

Subject to reporting requirements of United States SARA Section 313

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)

15.2. International regulations

CANADA

Tetrahydrofuran (109-99-9)

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)

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

EU-Regulations

Tetrahydrofuran (109-99-9)

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

Isopropanol (67-63-0)

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

National regulations

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Tetrahydrofuran (109-99-9)

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)

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)

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)

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

Tetrahydrofuran (109-99-9)

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

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

SECTION 16: Other information

Full text of H-phrases::

H225	Highly flammable liquid and vapor
H228	Flammable solid
H302	Harmful if swallowed
H314	Causes severe skin burns and eye damage
H318	Causes serious eye damage
H319	Causes serious eye irritation
H335	May cause respiratory irritation
H336	May cause drowsiness or dizziness
H351	Suspected of causing cancer

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

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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)
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.

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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

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