



TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M in hexane

Safety Data Sheet AKT851.1

Date of issue: 01/12/2015 Version: 1.0

SECTION 1: Identification

1.1. Identification

Product name	: TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M in hexane
Product code	: AKT851.1
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

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	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
Reproductive toxicity Category 2	H361 Suspected of damaging fertility or the unborn child
Specific target organ toxicity (single exposure) Category 3	H336 May cause drowsiness or dizziness
Specific target organ toxicity (repeated exposure) Category 2	H373 May cause damage to organs through prolonged or repeated exposure
Hazardous to the aquatic environment - Chronic Hazard Category 2	H411 Toxic to aquatic life with long lasting effects

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
- H336 - May cause drowsiness or dizziness
- H361 - Suspected of damaging fertility or the unborn child
- H373 - May cause damage to organs through prolonged or repeated exposure
- H411 - Toxic to aquatic life with long lasting effects

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.
- 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.

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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
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
P308+P313 - If exposed or concerned: Get medical advice/attention.
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
Hexanes	(CAS-No.) 73513-42-5	< 45	Flam. Liq. 2, H225 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 Repr. 2, H361 STOT SE 3, H336 STOT RE 2, H373 Asp. Tox. 1, H304 Aquatic Chronic 2, H411
Isopropanol	(CAS-No.) 67-63-0	< 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. IF exposed or concerned: Get medical advice/attention.

First-aid measures after inhalation : Remove victim to fresh air and keep at rest in a position comfortable for breathing. Immediately call a poison center or doctor/physician.

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. Immediately call a poison center or doctor/physician.

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

Symptoms/effects : Causes severe skin burns and eye damage. Suspected of damaging fertility or the unborn child. Causes damage to organs.

Symptoms/effects after inhalation : May cause drowsiness or dizziness. May cause irritation to the respiratory tract. 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 fatal if swallowed and enters airways.

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.

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SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

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

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

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

Emergency procedures : Evacuate unnecessary personnel.

6.1.2. For emergency responders

Protective equipment : Equip cleanup crew with proper protection. Avoid breathing vapors.

6.2. Environmental precautions

Prevent entry to sewers and public waters. Notify authorities if liquid enters sewers or public waters. Avoid release to the environment.

6.3. Methods and material for containment and cleaning up

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.

Precautions for safe handling : Do not handle until all safety precautions have been read and understood. Obtain special instructions before use. Avoid all eye and skin contact and do not breathe vapor and mist. Containers and transfer lines require grounding during use. Provide good ventilation in process area to prevent accumulation of vapors. Use only outdoors or in a well-ventilated area. Use only non-sparking tools.

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

Technical measures : Ground/bond container and receiving equipment. Proper grounding procedures to avoid static electricity should be followed. Use explosion-proof electrical equipment.

Storage conditions : Keep container tightly closed.

Incompatible materials : Moist air. Oxidizing agent. Water.

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/m ³)	980 mg/m ³
OSHA	OSHA PEL (TWA) (ppm)	400 ppm
IDLH	US IDLH (ppm)	2000 ppm (10% LEL)
NIOSH	NIOSH REL (TWA) (mg/m ³)	980 mg/m ³
NIOSH	NIOSH REL (TWA) (ppm)	400 ppm
NIOSH	NIOSH REL (STEL) (mg/m ³)	1225 mg/m ³

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Isopropanol (67-63-0)		
NIOSH	NIOSH REL (STEL) (ppm)	500 ppm

Hexanes (73513-42-5)		
ACGIH	ACGIH TWA (ppm)	500 ppm
ACGIH	ACGIH STEL (ppm)	1000 ppm
NIOSH	NIOSH REL (TWA) (mg/m ³)	350 mg/m ³
NIOSH	NIOSH REL (TWA) (ppm)	100 ppm
NIOSH	NIOSH REL (ceiling) (mg/m ³)	1800 mg/m ³
NIOSH	NIOSH REL (ceiling) (ppm)	510 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:

Wear respiratory protection. 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	: No data available
Freezing point	: No data available
Boiling point	: 69 °C - initial (hexane)
Flash point	: -23 °C
Auto-ignition temperature	: 225 (hexane)
Decomposition temperature	: No data available
Flammability (solid, gas)	: Highly flammable liquid and vapor
Vapor pressure	: 100 mm Hg @ 15.8°C (hexane)
Relative vapor density at 20 °C	: > 1
Relative density	: 0.898
% Volatiles	: > 70 %
Solubility	: Reacts with water.
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: No data available
Viscosity, dynamic	: No data available

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Explosive properties : No data available
Oxidizing properties : No data available
Explosion limits : 1.2 - 7.5 vol % (lower; upper)

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

Moist air. Oxidizing agent. Water.

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/m ³ (Exposure time: 4 h)
ATE US (oral)	1870 mg/kg body weight
ATE US (dermal)	4059 mg/kg body weight

Hexanes (73513-42-5)

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

Isopropanol (67-63-0)

IARC group	3 - Not classifiable
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Reproductive toxicity : Suspected of damaging fertility or the unborn child.

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

Specific target organ toxicity – repeated exposure : May cause damage to organs through prolonged or repeated exposure.
May cause damage to organs through prolonged or repeated exposure

Aspiration hazard : Not classified

Symptoms/effects after inhalation : May cause drowsiness or dizziness. May cause irritation to the respiratory tract. 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 fatal if swallowed and enters airways.

SECTION 12: Ecological information

12.1. Toxicity

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

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])

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12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Isopropanol (67-63-0)

Log Pow	0.05 (at 25 °C)
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12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Effect on the ozone layer : No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

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) : 1993
DOT NA no. : UN1993

14.2. UN proper shipping name

Transport document description : UN1993 Flammable liquids, n.o.s. (TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M in hexane), 3, II

Proper Shipping Name (DOT) : Flammable liquids, n.o.s.
(TITANIUM CHLORIDE TRIISOPROPOXIDE, 2M in hexane)

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



Dangerous for the environment : Yes

Marine pollutant : Yes



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.

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.

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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

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)

Titanium chloride triisopropoxide (20717-86-6)

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

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)

Hexanes (73513-42-5)

WHMIS Classification

Class B Division 2 - Flammable Liquid

EU-Regulations

Isopropanol (67-63-0)

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)

Hexanes (73513-42-5)

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 NZIoC (New Zealand Inventory 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

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SECTION 16: Other information

Full text 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
H361	Suspected of damaging fertility or the unborn child
H373	May cause damage to organs through prolonged or repeated exposure
H411	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.: 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

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.

Date of issue: 01/12/2015 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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