

Safety Data Sheet AKZ947

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1. Product identifier

Product form : Mixture
Physical state : Liquid

Product name : ZIRCONIUM DI-n-BUTOXIDE BIS(2,4-PENTANEDIONATE), 25% in n-butanol/toluene

Product code : AKZ947
Formula : C18H32O6Zr

Synonyms : ZIRCONIUM ACETYLACETONATE BUTYLATE

Chemical family : METAL COMPOUND

1.2. Relevant identified uses of the substance or mixture and uses advised against

Use of the substance/mixture : Chemical intermediate

For research use only

1.3. Details of the supplier of the safety data sheet

GELEST, INC.

11 East Steel Road Morrisville, PA 19067

USA

T 215-547-1015 - F 215-547-2484 - (M-F): 8:00 AM - 5:30 PM EST

info@gelest.com - www.gelest.com

1.4. Emergency telephone number

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

SECTION 2: Hazards identification

2.1. Classification of the substance or mixture

GHS-US classification

Flam. Liq. 3 H226 Skin Irrit. 2 H315 Eye Irrit. 2A H319 Repr. 2 H361 STOT SE 3 H335 STOT SE 3 H336 STOT RE 2 H373 Aquatic Acute 3 H402

Full text of H statements : see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US)







GHS02

GHS07

GHS08

Signal word (GHS-US) : Warning

Hazard statements (GHS-US) : H226 - Flammable liquid and vapor

H315 - Causes skin irritation
H319 - Causes serious eye irritation

H335 - May cause respiratory 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

H402 - Harmful to aquatic life

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

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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

P273 - Avoid release to the environment

P302+P352 - If on skin: Wash with plenty of water

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

P337+P313 - If eye irritation persists: Get medical advice/attention P308+P313 - If exposed or concerned: Get medical advice/attention

P314 - Get medical advice/attention if you feel unwell

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. Other hazards

No additional information available

Unknown acute toxicity (GHS US)

No data available

SECTION 3: Composition/Information on ingredients

Substance

Not applicable

3.2. **Mixture**

Name	Product identifier	%	GHS-US classification
Toluene	(CAS No) 108-88-3	46 - 54	Skin Irrit. 2, H315 Eye Irrit. 2A, H319 Repr. 2, H361 STOT SE 3, H336 STOT RE 2, H373 Asp. Tox. 1, H304
n-Butanol	(CAS No) 71-36-3	23 - 27	Flam. Liq. 3, H226 Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335
Zirconium di-n-butoxide bis(2,4-pentanedionate)	(CAS No) 62905-51-5	23 - 27	Eye Irrit. 2A, H319

SECTION 4: First aid measures

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 immediate medical advice/attention.

Most important symptoms and effects, both acute and delayed

Symptoms/injuries

: Suspected of damaging fertility or the unborn child. May cause damage to organs through prolonged or repeated exposure.

Symptoms/injuries after inhalation

May cause drowsiness or dizziness. May cause respiratory irritation. Toluene is moderately toxic by inhalation. Human systemic effects include CNS recording changes, hallucinations, distorted perceptions.

Symptoms/injuries after skin contact

: Causes skin irritation.

Symptoms/injuries after eye contact

: Causes serious eye irritation.

Symptoms/injuries after ingestion

May be harmful if swallowed. Oral toxicity is associated with toluene which causes psychophysiological and bone marrow changes nausea, vomiting, headache, visual effects including blindness.

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Chronic symptoms

NOTE: 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. n-butanol is metabolized to butanoic acid and 3hydroxybutanoic acid which may result in ketosis or ketoacidosis.

Indication of any immediate medical attention and special treatment needed

No additional information available

SECTION 5: Firefighting measures

Extinguishing media

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

Unsuitable extinguishing media : Do not use straight streams.

5.2. Special hazards arising from the substance or mixture

: Highly flammable liquid and vapor. Irritating fumes and organic acid vapors may develop when Fire hazard

material is exposed to elevated temperatures or open flame.

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

Advice for firefighters

Firefighting instructions : Exercise caution when fighting any chemical fire. Use water spray to cool exposed surfaces.

Do not enter fire area without proper protective equipment, including respiratory protection. Protection during firefighting

Avoid all eye and skin contact and do not breathe vapor and mist.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

: Eliminate every possible source of ignition. Use special care to avoid static electric charges. General measures

For non-emergency personnel 6.1.1.

Protective equipment Wear protective equipment as described in Section 8.

Emergency procedures Evacuate unnecessary personnel.

For emergency responders 6.1.2

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".

Environmental precautions

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

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

: Clean up any spills as soon as possible, using an absorbent material to collect it. Sweep or Methods for cleaning up

shovel spills into appropriate container for disposal. Use only non-sparking tools.

Reference to other sections

See Heading 8. Exposure controls and personal protection.

SECTION 7: Handling and storage

Precautions for safe handling

: Handle empty containers with care because residual vapors are flammable. Keep away from Additional hazards when processed

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. 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 contaminated clothing before reuse. Wash hands and other exposed areas with mild

soap and water before eating, drinking or smoking and when leaving work.

Conditions for safe storage, including any incompatibilities

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

electrical equipment.

Storage conditions : Keep container tightly closed. Keep in a cool place. Store locked up.

Incompatible materials

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

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7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Toluene (108-88-3)		
USA ACGIH	ACGIH TWA (ppm)	20 ppm
USA NIOSH	NIOSH REL (TWA) (mg/m³)	375 mg/m³
USA NIOSH	NIOSH REL (TWA) (ppm)	100 ppm
USA NIOSH	NIOSH REL (STEL) (mg/m³)	560 mg/m³
USA NIOSH	NIOSH REL (STEL) (ppm)	150 ppm
USA OSHA	OSHA PEL (TWA) (ppm)	200 ppm
USA OSHA	OSHA PEL (Ceiling) (ppm)	300 ppm
USA IDLH	US IDLH (ppm)	500 ppm

n-Butanol (71-36-3)			
USA ACGIH	ACGIH TWA (ppm)		20 ppm
USA NIOSH	NIOSH REL (ceiling) (mg/m³)	150 mg/m³
USA NIOSH	NIOSH REL (ceiling) (ppm)		50 ppm
USA OSHA	OSHA PEL (TWA) (mg/m³)		300 mg/m³
USA OSHA	OSHA PEL (TWA) (ppm)		100 ppm
USA IDLH	US IDLH (ppm)		1400 ppm (10% LEL)

Zirconium di-n-butoxide bis(2,4-pentanedionate) (62905-51-5)					
USA ACGIH	ACGIH TWA (mg/m³)		5 mg/m³ Zr		

8.2. Exposure controls

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

Personal protective equipment : Avoid all unnecessary exposure. Emergency eye wash fountains and safety showers should be available in the immediate vicinity of any potential exposure.

Hand protection : Neoprene or nitrile rubber gloves.

Eye protection : Chemical goggles. Contact lenses should not be worn.

Skin and body protection : Wear suitable protective clothing.

Respiratory protection : Where exposure through inhalation may occur from use, respiratory protection equipment is

recommended. NIOSH-certified organic vapor (black cartridge) respirator.

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

: Liquid Physical state Appearance : Liquid. Molecular mass : 435.66 g/mol Light amber. Color Characteristic. Odor Odor threshold No data available Refractive index : No data available pΗ No data available Relative evaporation rate (butyl acetate=1) No data available Melting point : No data available Freezing point : No data available : 117 °C - initial Boiling point Flash point 34 °C Auto-ignition temperature : 0

Decomposition temperature : No data available

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

Vapor pressure : 4 mm Hg @ 20°C

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Relative vapor density at 20 °C : 2.6 (n-butanol)
Relative density : 0.918

VOC content : > 70 °C

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 : 1.4 - 11.2 vol % (lower; upper: n-butanol)

9.2. Other information

No additional information available

SECTION 10: Stability and reactivity

10.1. Reactivity

No additional information available

10.2. Chemical stability

Stable.

10.3. Possibility of hazardous reactions

Material decomposes slowly in contact with water.

10.4. Conditions to avoid

Heat. Open flame. Sparks.

10.5. Incompatible materials

Water.

10.6. Hazardous decomposition products

Organic acid vapors. Zirconium oxide fumes.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Acute toxicity : Not classified

Toluene (108-88-3)		
LD50 oral rat	2600 mg/kg	
LD50 dermal rabbit	12000 mg/kg	
LC50 inhalation rat (mg/l)	12.5 mg/l/4h	

n-Butanol (71-36-3)	
LD50 oral rat	700 mg/kg
LD50 dermal rabbit	3402 mg/kg
LC50 inhalation rat (ppm)	> 8000 ppm/4h
ATE US (oral)	700.000 mg/kg body weight
ATE US (dermal)	3402.000 mg/kg body weight

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

|--|

IARC group 3 - Not classifiable

Reproductive toxicity : Suspected of damaging fertility or the unborn child.

Specific target organ toxicity (single exposure) : May cause respiratory irritation. May cause drowsiness or dizziness.

Specific target organ toxicity (repeated

exposure)

: May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard : Not classified

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Potential Adverse human health effects and	: Vapor inhalation of toluene may lead to impairment of coordination mental alertness, and
symptoms	reaction times. leading to assident property. Exposure to levels around 500ppm leads to

symptoms

reaction times, leading to accident proneness. Exposure to levels around 500ppm leads to narcotic effects including nausea, headache and mental confusion.

Symptoms/injuries after inhalation : May cause drowsiness or dizziness. May cause respiratory irritation. Toluene is moderately toxic by inhalation. Human systemic effects include CNS recording changes, hallucinations,

distorted perceptions.

Symptoms/injuries after skin contact : Causes skin irritation.

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

Symptoms/injuries after ingestion : May be harmful if swallowed. Oral toxicity is associated with toluene which causes

psychophysiological and bone marrow changes nausea, vomiting, headache, visual effects

including blindness.

Chronic symptoms : NOTE: 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. n-butanol is metabolized to butanoic acid and 3-

hydroxybutanoic acid which may result in ketosis or ketoacidosis.

Reason for classification : Expert judgment

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Harmful to aquatic life.

Toluene (108-88-3)	
LC50 fish 1	15.22 - 19.05 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
EC50 Daphnia 1	5.46 - 9.83 mg/l (Exposure time: 48 h - Species: Daphnia magna [Static])
LC50 fish 2	12.6 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])
EC50 Daphnia 2	11.5 mg/l (Exposure time: 48 h - Species: Daphnia magna)

n-Butanol (71-36-3)	
LC50 fish 1	1730 - 1910 mg/l (Exposure time: 96 h - Species: Pimephales promelas [static])
EC50 Daphnia 1	1983 mg/l (Exposure time: 48 h - Species: Daphnia magna)
LC50 fish 2	1740 mg/l (Exposure time: 96 h - Species: Pimephales promelas [flow-through])
EC50 Daphnia 2	1897 - 2072 mg/l (Exposure time: 48 h - Species: Daphnia magna [Static])

12.2. Persistence and degradability

No additional information available

12.3. Bioaccumulative potential

Toluene (108-88-3)	
Log Pow	2.65
n-Butanol (71-36-3)	
BCF fish 1	0.64
Log Pow	0.785 (at 25 °C)

12.4. Mobility in soil

No additional information available

12.5. Other adverse effects

Effect on ozone layer : No additional information available

Effect on the global warming : No known ecological damage caused by this product.

SECTION 13: Disposal considerations

13.1. Waste treatment methods

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

Waste disposal recommendations : Dispose in a safe manner in accordance with local/national regulations. Dispose of

contents/container to licensed waste disposal facility.

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

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14.2. UN proper shipping name

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

(ZIRCONIUM DI-n-BUTOXIDE BIS(2,4-PENTANEDIONATE), 25% in n-butanol/toluene)

Class (DOT) : 3 - Class 3 - Flammable and combustible liquid 49 CFR 173.120

Hazard labels (DOT) : 3 - Flammable liquid



DOT Symbols : G - Identifies PSN requiring a technical name

Packing group (DOT) : III - Minor Danger

DOT Packaging Exceptions (49 CFR 173.xxx) : 150
DOT Packaging Non Bulk (49 CFR 173.xxx) : 203
DOT Packaging Bulk (49 CFR 173.xxx) : 242

14.3. Additional information

Emergency Response Guide (ERG) Number : 128

Other information : No supplementary information available.

Transport by sea

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

passenger vessel

Air transport

DOT Quantity Limitations Passenger aircraft/rail : 60 L

(49 CFR 173.27)

DOT Quantity Limitations Cargo aircraft only (49 : 220 L

CFR 175.75)

SECTION 15: Regulatory information

15.1. US Federal regulations

ZIRCONIUM DI-n-BUTOXIDE BIS(2,4-PENTANEDIONATE), 25% in n-butanol/toluene		
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	

Toluene (108-88-3)
Listed on the United States TSCA (Toxic Substances Control Act) inventory
Subject to reporting requirements of United States SARA Section 313

SARA Section 313 - Emission Reporting 1.0 %

n-Butanol (71-36-3)

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 Section 4 test rule under TSCA Y2 - Y2 - indicates an exempt polymer that is a polyester and is made only from reactants included in a specified list of low concern reactants that comprises one of the eligibility criteria for the exemption rule
SARA Section 313 - Emission Reporting	1.0 %

Zirconium di-n-butoxide bis(2,4-pentanedionate) (62905-51-5)

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

15.2. International regulations

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Toluene (108-88-3)

Listed on the AICS (Australian Inventory of Chemical Substances)

Listed on the Canadian DSL (Domestic Substances List)

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

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

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)

Japanese Poisonous and Deleterious Substances Control Law

Japanese Pollutant Release and Transfer Register Law (PRTR Law)

Listed on the Canadian IDL (Ingredient Disclosure List)

Listed on INSQ (Mexican national Inventory of Chemical Substances)

Listed on Turkish inventory of chemical

n-Butanol (71-36-3)

Listed on the AICS (Australian Inventory of Chemical Substances)

Listed on the Canadian DSL (Domestic Substances List)

Listed on IECSC (Inventory of Existing Chemical Substances Produced or Imported in China)

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

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 Turkish inventory of chemical

Zirconium di-n-butoxide bis(2,4-pentanedionate) (62905-51-5)

15.3. US State regulations

15.3. US State regulations		15.3. US State regulations					
ZIRCONIUM DI-n-BUTOXIDE BIS(2,4-PENTANEDIONATE), 25% in n-butanol/toluene()							
U.S California - Proposition 65 - Carcinogens List		No					
U.S California - Proposition 65 - Developmental Toxicity		No					
U.S California - Proposition 65 - Reproductive Toxicity - Female		No					
U.S California - Proposition 65 - Reproductive Toxicity - Male		No					
Toluene (108-88-3)							
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	Non-significant risk level (NSRL)			
No	Yes	Yes	No				
n-Butanol (71-36-3)							
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	Non-significant risk level (NSRL)			
No	No	No	No				
Zirconium di-n-butoxide bis(2,4-pentanedionate) (62905-51-5)							
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	Non-significant risk level (NSRL)			
No	No	No	No				
n-Butanol (71-36-3)							

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SECTION 16: Other information

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.

Full text of H-phrases::

H226	Flammable liquid and vapor
H302	Harmful if swallowed
H304	May be fatal if swallowed and enters airways
H315	Causes skin irritation
H319	Causes serious eye irritation
H335	May cause respiratory 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
H402	Harmful to aquatic life

HMIS III Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 3 Serious Hazard
Physical : 1 Slight Hazard

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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