

ZIRCONIUM n-BUTOXIDE, 80% in n-butanol

Safety Data Sheet AKZ945
Date of issue: 06/30/2015 Version: 1.0

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 n-BUTOXIDE, 80% in n-butanol
Product code	: AKZ945
Formula	: C16H36O4Zr2
Synonyms	: ZIRCONIUM BUTYLATE; TETRABUTYL ZIRCONATE
Chemical family	: METAL ALCOHOLATE

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

Use of the substance/mixture	: Chemical intermediate For research and industrial use only
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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

Classification (GHS-US)

Flam. Liq. 3 H226
Skin Irrit. 2 H315
Eye Irrit. 2A H319
STOT SE 3 H335

Full text of H-phrases: see section 16

2.2. Label elements

GHS-US labeling

Hazard pictograms (GHS-US)



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

Precautionary statements (GHS-US)

: P280 - Wear protective gloves/protective clothing/eye protection/face protection

P210 - Keep away from heat, open flames, sparks. - No smoking

P233 - Keep container tightly closed

P240 - Ground/bond container and receiving equipment

P241 - Use explosion-proof electrical equipment

P242 - Use only non-sparking tools

P243 - Take precautionary measures against static discharge

P261 - Avoid breathing vapors

P264 - Wash hands thoroughly after handling

P271 - Use only outdoors or in a well-ventilated area

P304+P340 - If inhaled: Remove person to fresh air and keep comfortable for breathing

P303+P361+P353 - If on skin (or hair): take off immediately all contaminated clothing. Rinse skin with water/shower

P332+P313 - If skin irritation occurs: Get medical advice/attention

P305+P351+P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing

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P337+P313 - If eye irritation persists: Get medical advice/attention
P312 - Call a doctor if you feel unwell
P362 - Take off contaminated clothing and wash before reuse
P370+P378 - In case of fire: Use dry chemical, dry soda ash 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

Other hazards not contributing to the classification

: Material may form zirconium oxides or zirconate polymers on the skin, eyes or in the lungs. Prolonged exposure to zirconium compounds can induce formation of granulomatous lesions in the lungs or on the skin. n-butanol is metabolized to butanoic acid and 3-hydroxybutanoic acid which result in ketosis or ketoacidosis.

2.4. Unknown acute toxicity (GHS US)

No data available

SECTION 3: Composition/information on ingredients

3.1. Substance

Not applicable

3.2. Mixture

Name	Product identifier	%	Classification (GHS-US)
Zirconium n-butoxide	(CAS No) 1071-76-7	> 75	Flam. Liq. 3, H226 Skin Irrit. 2, H315 Eye Irrit. 2A, H319
n-Butanol	(CAS No) 71-36-3	> 20	Flam. Liq. 3, H226 Acute Tox. 4 (Oral), H302 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 STOT SE 3, H335

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 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, both acute and delayed

Symptoms/injuries after inhalation

: May cause respiratory irritation. May cause drowsiness or dizziness.

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.

4.3. Indication of any immediate medical attention and special treatment needed

No additional information available

SECTION 5: Firefighting measures

5.1. Extinguishing media

Suitable extinguishing media

: Water spray. Foam. Carbon dioxide. Dry chemical.

Unsuitable extinguishing media

: None known.

5.2. Special hazards arising from the substance or mixture

Fire hazard

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

5.3. Advice for firefighters

Firefighting instructions

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

Protection during firefighting

: Do not enter fire area without proper protective equipment, including respiratory protection. Wear pressure demand self-contained breathing apparatus with full facepiece and full protective clothing. Avoid all eye and skin contact and do not breathe vapor and mist.

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SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

General measures : Remove ignition sources. 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.

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

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

Precautions for safe handling : Avoid all eye and skin contact and do not breathe vapor and mist. Containers must be properly grounded before beginning transfer. Provide good ventilation in process area to prevent accumulation of vapors. 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

: Water.

Storage area

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

7.3. Specific end use(s)

No additional information available

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

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

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 caustic 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 : 383.68 g/mol

Color : Light. Amber.

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Odor	: Characteristic.
Odor threshold	: No data available
Refractive index	: 1.4565
pH	: No data available
Relative evaporation rate (butyl acetate=1)	: No data available
Melting point	: No data available
Freezing point	: -21 °C
Boiling point	: 117 °C (initial, n-butanol)
Flash point	: 34 °C
Auto-ignition temperature	: No data available
Decomposition temperature	: No data available
Flammability (solid, gas)	: Flammable liquid and vapor
Vapor pressure	: 4 mm Hg @ 20°C
Relative vapor density at 20 °C	: > 1
Relative density	: 1.07
VOC content	: > 20 %
Solubility	: Reacts with water.
Log Pow	: No data available
Log Kow	: No data available
Viscosity, kinematic	: 120 - 160
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

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

Reproductive toxicity : Not classified

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Specific target organ toxicity (single exposure)	: May cause respiratory irritation.
Specific target organ toxicity (repeated exposure)	: Not classified
Aspiration hazard	: Not classified
Symptoms/injuries after inhalation	: May cause respiratory irritation. May cause drowsiness or dizziness.
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.
Reason for classification	: Expert judgment

SECTION 12: Ecological information

12.1. Toxicity

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

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

Other adverse effects	: This substance may be hazardous to the environment.
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

Waste disposal recommendations	: Dispose in a safe manner in accordance with local/national regulations. Dispose of contents/container to licensed waste disposal facility.
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

Proper Shipping Name (DOT)	: Flammable liquids, n.o.s. (ZIRCONIUM n-BUTOXIDE, 80% in n-butanol)
Department of Transportation (DOT) Hazard Classes	: 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

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14.3. Additional information

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 CFR 175.75) : 220 L

SECTION 15: Regulatory information

15.1. US Federal regulations

n-Butanol (71-36-3)

Listed on the United States TSCA (Toxic Substances Control Act) inventory
Listed on 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.
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SARA Section 313 - Emission Reporting

1.0 %

Zirconium n-butoxide (1071-76-7)

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

15.2. International regulations

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

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Listed on the AICS (Australian Inventory of Chemical Substances)
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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)

15.3. US State regulations

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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

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	No significance risk level (NSRL)
No	No	No	No	

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Zirconium n-butoxide (1071-76-7)				
U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No significance risk level (NSRL)
No	No	No	No	

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.: 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.

Full text of H-phrases::

Acute Tox. 4 (Oral)	Acute toxicity (oral) Category 4
Eye Irrit. 2A	Serious eye damage/eye irritation Category 2A
Flam. Liq. 3	Flammable liquids Category 3
Skin Irrit. 2	Skin corrosion/irritation Category 2
STOT SE 3	Specific target organ toxicity (single exposure) Category 3
H226	Flammable liquid and vapor
H302	Harmful if swallowed
H315	Causes skin irritation
H319	Causes serious eye irritation
H335	May cause respiratory irritation

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.

Date of issue: 06/30/2015 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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