

SAFETY DATA SHEET

Version 6.5
Revision Date 03/02/2024
Print Date 04/28/2024

SECTION 1: Identification of the substance/mixture and of the company/undertaking**1.1 Product identifiers**

Product name : Zirconium(IV) butoxide solution

Product Number : 333948
Brand : Aldrich

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

Identified uses : Laboratory chemicals, Synthesis of substances

Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATES

Telephone : +1 314 771-5765
Fax : +1 800 325-5052

1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2: Hazards identification**2.1 Classification of the substance or mixture****GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)**

Flammable liquids (Category 3), H226
Skin corrosion (Category 1B), H314
Serious eye damage (Category 1), H318
Specific target organ toxicity - single exposure (Category 3), Respiratory system, Central nervous system, H335, H336

For the full text of the H-Statements mentioned in this Section, see Section 16.

2.2 GHS Label elements, including precautionary statements

Pictogram



Signal Word

Danger

Hazard Statements

H226

Flammable liquid and vapor.

H314

Causes severe skin burns and eye damage.

H335

May cause respiratory irritation.

H336

May cause drowsiness or dizziness.

Precautionary Statements

P210

Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.

P233

Keep container tightly closed.

P240

Ground/bond container and receiving equipment.

P241

Use explosion-proof electrical/ ventilating/ lighting/ equipment.

P242

Use only non-sparking tools.

P243

Take precautionary measures against static discharge.

P261

Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.

P264

Wash skin thoroughly after handling.

P271

Use only outdoors or in a well-ventilated area.

P280

Wear protective gloves/ protective clothing/ eye protection/ face protection.

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 + P310

IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER/ doctor.

P305 + P351 + P338 +
P310

IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing. Immediately call a POISON CENTER/ doctor.

P363

Wash contaminated clothing before reuse.

P370 + P378

In case of fire: Use dry sand, dry chemical or alcohol-resistant foam to extinguish.

P403 + P233

Store in a well-ventilated place. Keep container tightly closed.

P403 + P235

Store in a well-ventilated place. Keep cool.

P405

Store locked up.

P501

Dispose of contents/ container to an approved waste disposal plant.

2.3 Hazards not otherwise classified (HNOC) or not covered by GHS - none

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Synonyms : Tetrabutyl zirconatesolution

Formula : $C_{16}H_{36}O_4Zr$

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Molecular weight : 383.68 g/mol

Component		Classification	Concentration
zirconium tetrabutanolate			
CAS-No.	1071-76-7	Flam. Liq. 3; Skin Corr. 1B; Eye Dam. 1; H226, H314, H318	>= 70 - < 90 %
EC-No.	213-995-3		
n-butanol			
CAS-No.	71-36-3	Flam. Liq. 3; Acute Tox. 4; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; H226, H302, H315, H318, H335, H336 Concentration limits: >= 20 %: STOT SE 3, H335; >= 20 %: STOT SE 3, H336;	>= 20 - < 30 %
EC-No.	200-751-6		
Index-No.	603-004-00-6		
Registration number	01-2119484630-38-XXXX		

For the full text of the H-Statements mentioned in this Section, see Section 16.

SECTION 4: First aid measures

4.1 Description of first-aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor in attendance.

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

4.2 Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

4.3 Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

5.1 Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

5.2 Special hazards arising from the substance or mixture

Carbon oxides

Zirconium oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air at elevated temperatures.

Development of hazardous combustion gases or vapours possible in the event of fire.

5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition.

Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

6.2 Environmental precautions

Do not let product enter drains. Risk of explosion.

6.3 Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemisorb®).

Dispose of properly. Clean up affected area.

6.4 Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.

Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities

Storage conditions

Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.

Moisture sensitive.

Storage class

Storage class (TRGS 510): 3: Flammable liquids

7.3 Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
zirconium tetrabutanolate	1071-76-7	TWA	5 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		TWA	5 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Not classifiable as a human carcinogen		
		STEL	10 mg/m ³	USA. ACGIH Threshold Limit Values (TLV)
		Not classifiable as a human carcinogen		

		TWA	5 mg/m3	USA. NIOSH Recommended Exposure Limits
		ST	10 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	5 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		STEL	10 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
n-butanol	71-36-3	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		C	50 ppm 150 mg/m3	USA. NIOSH Recommended Exposure Limits
		Potential for dermal absorption		
		TWA	100 ppm 300 mg/m3	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		C	50 ppm 150 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)
		Skin		

8.2 Exposure controls

Appropriate engineering controls

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

Recommended Filter type: Filter type ABEK

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

required when vapours/aerosols are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Control of environmental exposure

Do not let product enter drains. Risk of explosion.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

- | | |
|---|---|
| a) Appearance | Form: cloudy, liquid
Color: colorless |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | No data available |
| f) Initial boiling point and boiling range | No data available |
| g) Flash point | 38 °C (100 °F) - closed cup |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | Upper explosion limit: 11.2 %(V)
Lower explosion limit: 1.4 %(V) |

k)	Vapor pressure	No data available
l)	Vapor density	No data available
m)	Density	1.049 g/cm ³
	Relative density	No data available
n)	Water solubility	No data available
o)	Partition coefficient: n-octanol/water	No data available
p)	Autoignition temperature	No data available
q)	Decomposition temperature	No data available
r)	Viscosity	No data available
s)	Explosive properties	Not classified as explosive.
t)	Oxidizing properties	none

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapor/air-mixtures are explosive at intense warming.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heating.

10.5 Incompatible materials

Bases, Oxidizing agents, Alkali metals, Strong oxidizing agents, Strong acids, Halogens

10.6 Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Mixture

Acute toxicity

Oral: No data available

Acute toxicity estimate Oral - 3,950 mg/kg
(Calculation method)

Symptoms: If ingested, severe burns of the mouth and throat, as well as a danger of perforation of the esophagus and the stomach.

Inhalation: No data available

Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Dermal: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)

Skin corrosion/irritation

Remarks: Mixture causes burns.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye damage.

Risk of blindness!

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Mixture may cause respiratory irritation.

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Central nervous system depression, Gastrointestinal disturbance, drying, cracking of the skin, Skin irritation
Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Components

zirconium tetrabutanolate

Acute toxicity

Oral: No data available

Inhalation: Corrosive to respiratory system.

Dermal: No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

Remarks: Causes serious eye damage.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

n-butanol

Acute toxicity

LD50 Oral - Rat - 790 mg/kg

Remarks: Liver:Fatty liver degeneration.

Kidney, Ureter, Bladder:Other changes.

Blood:Other changes.

(RTECS)

Inhalation: No data available

LD50 Dermal - Rabbit - male - 3,430 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 2 h

Remarks: (ECHA)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irreversible effects on the eye
(OECD Test Guideline 405)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): micronucleus.

Test system: Chinese hamster lung cells

Result: negative

Remarks: (ECHA)

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster lung cells

Result: negative

Method: OECD Test Guideline 474

Species: Mouse - male and female

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation. - Respiratory Tract, Skin, Eyes

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

May cause drowsiness or dizziness.

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

SECTION 12: Ecological information**12.1 Toxicity****Mixture**

No data available

12.2 Persistence and degradability

No data available

12.3 Bioaccumulative potential

No data available

12.4 Mobility in soil

No data available

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12.5 Results of PBT and vPvB assessment

PBT/vPvB assessment not available as chemical safety assessment not required/not conducted

12.6 Endocrine disrupting properties

No data available

12.7 Other adverse effects

No data available

Components

zirconium tetrabutanolate

No data available

n-butanol

Toxicity to fish	static test LC50 - Pimephales promelas (fathead minnow) - 1,376 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 1,328 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata (green algae) - 225 mg/l - 96 h (OECD Test Guideline 201)
Toxicity to bacteria	static test EC50 - Pseudomonas putida - 4,390 mg/l - 17 h (DIN 38421 TEIL 8)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	semi-static test EC50 - Daphnia magna (Water flea) - 18 mg/l - 21 d (OECD Test Guideline 211)

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself. See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

SECTION 14: Transport information

DOT (US)

UN number: 1993 Class: 3 Packing group: III
Proper shipping name: Flammable liquids, n.o.s. (zirconium tetrabutanolate, n-butanol)
Reportable Quantity (RQ): 100 lbs
Reportable Quantity (RQ):
Poison Inhalation Hazard: No

IMDG

UN number: 1993 Class: 3 Packing group: III EMS-No: F-E, S-E
Proper shipping name: FLAMMABLE LIQUID, N.O.S. (zirconium tetrabutanolate, n-butanol)

IATA

UN number: 1993 Class: 3 Packing group: III
Proper shipping name: Flammable liquid, n.o.s. (zirconium tetrabutanolate, n-butanol)

SECTION 15: Regulatory information

SARA 302 Components

This material does not contain any components with a section 302 EHS TPQ.

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Acute Health Hazard, Chronic Health Hazard

Reportable Quantity : F003 lbs

Massachusetts Right To Know Components

n-butanol	CAS-No. 71-36-3	Revision Date 2020-07-14
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Pennsylvania Right To Know Components

n-butanol	CAS-No. 71-36-3	Revision Date 2020-07-14
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SECTION 16: Other information

Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its

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