

SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

1.1. Product identifier

Product Description:	<u>Zirconium tert-butoxide</u>
Cat No. :	39547
CAS No	2081-12-1
Molecular Formula	C ₁₆ H ₃₆ O ₄ Zr
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

1.3. Details of the supplier of the safety data sheet

Company	Avocado Research Chemicals Ltd. (Part of Thermo Fisher Scientific) Shore Road, Heysham Lancashire, LA3 2XY, United Kingdom Office Tel: +44 (0) 1524 850506 Office Fax: +44 (0) 1524 850608
E-mail address	begel.sdsdesk@thermofisher.com

1.4. Emergency telephone number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

SECTION 2: HAZARDS IDENTIFICATION

2.1. Classification of the substance or mixture

CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

Physical hazards

Flammable liquids

Category 3 (H226)

Health hazards

Based on available data, the classification criteria are not met

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Environmental hazards

Based on available data, the classification criteria are not met

Full text of Hazard Statements: see section 16

2.2. Label elements



Signal Word

Warning

Hazard Statements

H226 - Flammable liquid and vapor

Precautionary Statements

P403 + P233 - Store in a well-ventilated place. Keep container tightly closed

P303 + P361 + P353 - IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower

P210 - Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking

2.3. Other hazards

This product does not contain any known or suspected endocrine disruptors

SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS

3.1. Substances

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
2-Propanol, 2-methyl-, zirconium(4+) salt (4:1)	2081-12-1		99.95	Flam. Liq. 3 (H226)

REACH registration number

-

Full text of Hazard Statements: see section 16

SECTION 4: FIRST AID MEASURES

4.1. Description of first aid measures

General Advice

If symptoms persist, call a physician.

Eye Contact

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

Skin Contact

Wash off immediately with plenty of water for at least 15 minutes. If skin irritation persists,

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	call a physician.
Ingestion	Clean mouth with water and drink afterwards plenty of water.
Inhalation	Remove to fresh air. If not breathing, give artificial respiration. Get medical attention if symptoms occur.
Self-Protection of the First Aider	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination.

4.2. Most important symptoms and effects, both acute and delayed

Difficulty in breathing. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting

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

Notes to Physician Treat symptomatically.

SECTION 5: FIREFIGHTING MEASURES

5.1. Extinguishing media

Suitable Extinguishing Media

Carbon dioxide (CO₂). Dry chemical. Chemical foam. Water mist may be used to cool closed containers. CO₂, dry chemical, dry sand, alcohol-resistant foam.

Extinguishing media which must not be used for safety reasons

Water.

5.2. Special hazards arising from the substance or mixture

Flammable. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Reacts violently with water.

Hazardous Combustion Products

Carbon monoxide (CO), Carbon dioxide (CO₂).

5.3. Advice for firefighters

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

SECTION 6: ACCIDENTAL RELEASE MEASURES

6.1. Personal precautions, protective equipment and emergency procedures

Ensure adequate ventilation. Use personal protective equipment as required. Remove all sources of ignition. Take precautionary measures against static discharges.

6.2. Environmental precautions

Should not be released into the environment. See Section 12 for additional Ecological Information.

6.3. Methods and material for containment and cleaning up

Keep in suitable, closed containers for disposal. Soak up with inert absorbent material. Do not expose spill to water. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment.

6.4. Reference to other sections

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Refer to protective measures listed in Sections 8 and 13.

SECTION 7: HANDLING AND STORAGE

7.1. Precautions for safe handling

Do not get in eyes, on skin, or on clothing. Wear personal protective equipment/face protection. Ensure adequate ventilation. Avoid ingestion and inhalation. Do not allow contact with water. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Take precautionary measures against static discharges.

Hygiene Measures

Handle in accordance with good industrial hygiene and safety practice. Keep away from food, drink and animal feeding stuffs. Do not eat, drink or smoke when using this product. Remove and wash contaminated clothing and gloves, including the inside, before re-use. Wash hands before breaks and after work.

7.2. Conditions for safe storage, including any incompatibilities

Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Keep away from heat, sparks and flame. Corrosives area. Store under an inert atmosphere. Material darkens in color during storage. Keep container tightly closed in a dry and well-ventilated place. Keep away from water or moist air.

Technical Rules for Hazardous Substances (TRGS) 510 Class 3
Storage Class (LGK) (Germany)

7.3. Specific end use(s)

Use in laboratories

SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

8.1. Control parameters

Exposure limits

List source(s): **UK** - EH40/2005 Work Exposure Limits, Fourth edition. Published 2020.

Component	The United Kingdom	European Union	Ireland
2-Propanol, 2-methyl-, zirconium(4+) salt (4:1)	STEL: 10 mg/m ³ 15 min TWA: 5 mg/m ³ 8 hr		

Biological limit values

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)

No information available

Predicted No Effect Concentration (PNEC)

No information available.

8.2. Exposure controls

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Engineering Measures

Use explosion-proof electrical/ventilating/lighting equipment. Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas.

Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source

Personal protective equipment

Eye Protection

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

Hand Protection

Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Disposable gloves	See manufacturers recommendations	-	EN 374	(minimum requirement)

Skin and body protection

Long sleeved clothing.

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatability, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

Respiratory Protection

No protective equipment is needed under normal use conditions.

Large scale/emergency use

Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced

Small scale/Laboratory use

Maintain adequate ventilation

Environmental exposure controls

No information available.

SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

9.1. Information on basic physical and chemical properties

Physical State	Liquid	
Appearance	Yellow	
Odor	No information available	
Odor Threshold	No data available	
Melting Point/Range	No data available	
Softening Point	No data available	
Boiling Point/Range	70 °C / 158 °F	@ 2 mmHg
Flammability (liquid)	Flammable	On basis of test data
Flammability (solid,gas)	Not applicable	Liquid
Explosion Limits	No data available	
Flash Point	55 °C / 131 °F	Method - No information available
Autoignition Temperature	No data available	
Decomposition Temperature	No data available	
pH	No information available	
Viscosity	No data available	
Water Solubility	decomposes	
Solubility in other solvents	No information available	
Partition Coefficient (n-octanol/water)		
Vapor Pressure	No data available	
Density / Specific Gravity	0.960	
Bulk Density	Not applicable	Liquid
Vapor Density	No data available	(Air = 1.0)

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Particle characteristics Not applicable (liquid)

9.2. Other information

Molecular Formula C16 H36 O4 Zr
Molecular Weight 383.68
Explosive Properties Vapors may form explosive mixtures with air explosive air/vapour mixtures possible

SECTION 10: STABILITY AND REACTIVITY

10.1. Reactivity
None known, based on information available

10.2. Chemical stability
Moisture sensitive. Light sensitive.

10.3. Possibility of hazardous reactions

Hazardous Polymerization No information available.
Hazardous Reactions None under normal processing. Reacts violently with water.

10.4. Conditions to avoid
Keep away from open flames, hot surfaces and sources of ignition. Exposure to light.
Incompatible products. Exposure to moist air or water. Exposure to moisture.

10.5. Incompatible materials
Strong oxidizing agents.

10.6. Hazardous decomposition products
Carbon monoxide (CO). Carbon dioxide (CO₂).

SECTION 11: TOXICOLOGICAL INFORMATION

11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008

Product Information No acute toxicity information is available for this product

(a) acute toxicity;
Oral No data available
Dermal No data available
Inhalation No data available

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;
Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

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(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Other Adverse Effects The toxicological properties have not been fully investigated.

Symptoms / effects, both acute and delayed Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

11.2. Information on other hazards

Endocrine Disrupting Properties Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.

SECTION 12: ECOLOGICAL INFORMATION

12.1. Toxicity

Ecotoxicity effects Do not empty into drains.

12.2. Persistence and degradability

Persistence Persistence is unlikely, based on information available.

12.3. Bioaccumulative potential

Bioaccumulation is unlikely

12.4. Mobility in soil

The product contains volatile organic compounds (VOC) which will evaporate easily from all surfaces. Will likely be mobile in the environment due to its volatility. Disperses rapidly in air.

12.5. Results of PBT and vPvB assessment

No data available for assessment.

12.6. Endocrine disrupting properties

Endocrine Disruptor Information This product does not contain any known or suspected endocrine disruptors

12.7. Other adverse effects Persistent Organic Pollutant Ozone Depletion Potential

This product does not contain any known or suspected substance
This product does not contain any known or suspected substance

SECTION 13: DISPOSAL CONSIDERATIONS

13.1. Waste treatment methods

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Waste from Residues/Unused Products	Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.
Contaminated Packaging	Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.
European Waste Catalogue (EWC)	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
Other Information	Waste codes should be assigned by the user based on the application for which the product was used. Do not flush to sewer. Can be landfilled or incinerated, when in compliance with local regulations.

SECTION 14: TRANSPORT INFORMATION

IMDG/IMO

14.1. UN number	UN2924
14.2. UN proper shipping name	FLAMMABLE LIQUID, CORROSIVE, N.O.S.
Technical Shipping Name	Zirconium tert-butoxide
14.3. Transport hazard class(es)	3
Subsidiary Hazard Class	8
14.4. Packing group	II

ADR

14.1. UN number	UN2924
14.2. UN proper shipping name	FLAMMABLE LIQUID, CORROSIVE, N.O.S.
Technical Shipping Name	Zirconium tert-butoxide
14.3. Transport hazard class(es)	3
Subsidiary Hazard Class	8
14.4. Packing group	II

IATA

14.1. UN number	UN2924
14.2. UN proper shipping name	FLAMMABLE LIQUID, CORROSIVE, N.O.S.
Technical Shipping Name	Zirconium tert-butoxide
14.3. Transport hazard class(es)	3
Subsidiary Hazard Class	8
14.4. Packing group	II

14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required.
14.7. Maritime transport in bulk according to IMO instruments	Not applicable, packaged goods

SECTION 15: REGULATORY INFORMATION

15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

International Inventories

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia

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(AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
2-Propanol, 2-methyl-, zirconium(4+) salt (4:1)	2081-12-1	-	-	-	-	X	KE-04174	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
2-Propanol, 2-methyl-, zirconium(4+) salt (4:1)	2081-12-1	-	-	-	-	-	X	-

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
2-Propanol, 2-methyl-, zirconium(4+) salt (4:1)	2081-12-1	-	Use restricted. See item 75. (see link for restriction details)	-

REACH links

<https://echa.europa.eu/substances-restricted-under-reach>

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
2-Propanol, 2-methyl-, zirconium(4+) salt (4:1)	2081-12-1	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

Water endangering class = 3 (self classification)

15.2. Chemical safety assessment

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A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H226 - Flammable liquid and vapor

Legend

CAS - Chemical Abstracts Service

EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

PICCS - Philippines Inventory of Chemicals and Chemical Substances

IECSC - Chinese Inventory of Existing Chemical Substances

KECL - Korean Existing and Evaluated Chemical Substances

TSCA - United States Toxic Substances Control Act Section 8(b) Inventory

DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List

ENCS - Japanese Existing and New Chemical Substances

AICS - Australian Inventory of Chemical Substances

NZIoC - New Zealand Inventory of Chemicals

WEL - Workplace Exposure Limit

ACGIH - American Conference of Governmental Industrial Hygienists

DNEL - Derived No Effect Level

RPE - Respiratory Protective Equipment

LC50 - Lethal Concentration 50%

NOEC - No Observed Effect Concentration

PBT - Persistent, Bioaccumulative, Toxic

TWA - Time Weighted Average

IARC - International Agency for Research on Cancer
Predicted No Effect Concentration (PNEC)

LD50 - Lethal Dose 50%

EC50 - Effective Concentration 50%

POW - Partition coefficient Octanol:Water

vPvB - very Persistent, very Bioaccumulative

ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road

IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code

OECD - Organisation for Economic Co-operation and Development

BCF - Bioconcentration factor

Key literature references and sources for data

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

ICAO/IATA - International Civil Aviation Organization/International Air Transport Association

MARPOL - International Convention for the Prevention of Pollution from Ships

ATE - Acute Toxicity Estimate

VOC - (Volatile Organic Compound)

Training Advice

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

Prepared By

Health, Safety and Environmental Department

Revision Date

10-Feb-2024

Revision Summary

New emergency telephone response service provider.

This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of Safety Data Sheet