

SAFETY DATA SHEET

Version 6.10
Revision Date 06/30/2021
Print Date 04/05/2022

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

Product name : Titanium(IV) butoxide

Product Number : 244112
Brand : Aldrich
CAS-No. : 5593-70-4

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

Identified uses : Laboratory chemicals, Synthesis of substances

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Quimica S de RL de CV
Parque Industrial Toluca 2000
Calle 6 Norte No. 107
50200 TOLUCA
MEXICO

Telephone : +52 (0)1 800 007 5300
Fax : +52 (0)1 800 712 9920

1.4 Emergency telephone

Emergency Phone # : 800-00-214-00 (SETIQ)
800-681-9531 (CHEMTREC)
(55) 55-59-15-88

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 irritation (Category 2), H315
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

Aldrich - 244112

Page 1 of 13

Hazard statement(s)	
H226	Flammable liquid and vapor.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H335	May cause respiratory irritation.
H336	May cause drowsiness or dizziness.
Precautionary statement(s)	
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/ eye protection/ face protection.
P303 + P361 + P353	IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340 + P312	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Call a POISON CENTER/ doctor if you feel unwell.
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.
P332 + P313	If skin irritation occurs: Get medical advice/ attention.
P362	Take off contaminated clothing and wash 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

Formula : $C_{16}H_{36}O_4Ti$
Molecular weight : 340.32 g/mol

Component		Classification	Concentration
titanium tetrabutanolate			
CAS-No.	5593-70-4	Flam. Liq. 3; Skin Irrit. 2; Eye Dam. 1; STOT SE 3; H226, H315, H318, H335, H336	>= 90 - <= 100 %
EC-No.	227-006-8		
Registration number	01-2119967423-33-XXXX		

titanium tetraisopropanolate			
CAS-No.	546-68-9	Flam. Liq. 3; Eye Irrit. 2A; STOT SE 3; H226, H319, H336	$\geq 5 - < 10$ %
EC-No.	208-909-6		
Registration number	01-2119967389-17-XXXX		
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	$\geq 1 - < 5$ %
EC-No.	200-751-6		
Index-No.	603-004-00-6		
Registration number	01-2119484630-38-XXXX	Concentration limits: ≥ 20 %: STOT SE 3, H335; ≥ 20 %: STOT SE 3, H336;	

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

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.

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: immediately make victim drink water (two glasses at most). Consult a physician.

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

Titanium/titanium oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Risk of dust explosion.

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. Chemizorb®).

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.

Air and moisture sensitive.
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
n-butanol	71-36-3	TWA	20 ppm	USA. ACGIH Threshold Limit Values (TLV)
		C	50 ppm 150 mg/m ³	USA. NIOSH Recommended Exposure Limits
	Remarks	Potential for dermal absorption		
		TWA	100 ppm 300 mg/m ³	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		C	50 ppm 150 mg/m ³	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

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: KCL 898 Butoject®

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact
Material: Nitrile rubber
Minimum layer thickness: 0.4 mm
Break through time: 30 min
Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

Body Protection

Flame retardant antistatic protective clothing.

Respiratory protection

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: liquid
Color: light yellow |
| b) Odor | No data available |
| c) Odor Threshold | No data available |
| d) pH | No data available |
| e) Melting point/freezing point | Melting point/range: < -75 °C (< -103 °F) - OECD Test Guideline 102 |
| f) Initial boiling point and boiling range | 206 °C 403 °F at 13 hPa - lit. |
| g) Flash point | 42 °C (108 °F) - Pensky-Martens closed cup - ASTM D 93 |
| h) Evaporation rate | No data available |
| i) Flammability (solid, gas) | No data available |
| j) Upper/lower flammability or explosive limits | No data available |
| k) Vapor pressure | No data available |
| l) Vapor density | No data available |
| m) Relative density | 0.99 at 25 °C (77 °F) |
| 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 No data available
- t) Oxidizing properties No data available

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 and 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 - 2,893 mg/kg

(Calculation method)

Symptoms: Irritations of mucous membranes in the mouth, pharynx, oesophagus and gastrointestinal tract.

Inhalation: No data available

Symptoms: Possible 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

Mixture causes skin irritation.

Serious eye damage/eye irritation

Mixture causes serious eye damage.

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

RTECS: XR1585000

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Stomach - Irregularities - Based on Human Evidence

Components**titanium tetrabutanolate****Acute toxicity**

LD50 Oral - Rat - 3,122 mg/kg

Remarks: (RTECS)

Inhalation: No data available

Dermal: No data available

Skin corrosion/irritation

Causes skin irritation. (ECHA)

Serious eye damage/eye irritation

Causes serious eye damage. (ECHA)

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

Test Type: Ames test

Test system: Escherichia coli/Salmonella typhimurium

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Human lymphocytes

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause respiratory irritation.

Skin contact - May cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

titanium tetraisopropanolate**Acute toxicity**

LD50 Oral - Rat - male - 7,500 mg/kg

Remarks: (ECHA)

Inhalation: No data available

Symptoms: Possible damages:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 24 h

Remarks: (ECHA)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation

(OECD Test Guideline 405)

Respiratory or skin sensitization

Local lymph node assay (LLNA) - Mouse

Result: negative

(Regulation (EC) No. 440/2008, Annex, B.42 (LLNA))

Germ cell mutagenicity

Test Type: Ames test

Test system: S. typhimurium

Result: negative

Method: US-EPA

Species: Mouse - male and female - Bone marrow

Result: negative

Remarks: (in analogy to similar products)

The value is given in analogy to the following substances: 2-Propanol

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause drowsiness or dizziness.

Acute inhalation toxicity - Possible damages:, mucosal irritations

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)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 2 h

Remarks: (ECHA)

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

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Irreversible effects on the eye

(OECD Test Guideline 405)

(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.

May cause drowsiness or dizziness.

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

12.5 Results of PBT and vPvB assessment

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

12.6 Other adverse effects

No data available

Components

titanium tetrabutanolate

No data available

titanium tetraisopropanolate

Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 590 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 820 mg/l - 72 h (OECD Test Guideline 201)
Toxicity to bacteria	EC50 - Bacteria - 1,050 mg/l - 16 h

n-butanol

Aldrich - 244112

Page 11 of 13

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)

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. (tetra-n-butyl orthotitanate, titanium tetraisopropanolate)
 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. (tetra-n-butyl orthotitanate, titanium tetraisopropanolate)

IATA

UN number: 1993 Class: 3 Packing group: III
 Proper shipping name: Flammable liquid, n.o.s. (tetra-n-butyl orthotitanate, titanium tetraisopropanolate)

SECTION 15: Regulatory information

SARA 302 Components

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

SARA 313 Components

The following components are subject to 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**

No components are subject to the Massachusetts Right to Know Act.

SECTION 16: Other information**Further information**

The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See www.sigma-aldrich.com and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact mlsbranding@sial.com.

Version: 6.10

Revision Date: 06/30/2021

Print Date: 04/05/2022