

SAFETY DATA SHEET

Version 6.6
Revision Date 03/05/2021
Print Date 09/25/2021**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : Titanium(IV) butoxide

Product Number : 86910
Brand : Sigma-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 sheetCompany : Sigma-Aldrich Inc.
3050 SPRUCE ST
ST. LOUIS MO 63103
UNITED STATESTelephone : +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 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

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

Synonyms : TYZOR® TBT organic titanate
Tetrabutyl orthotitanate
Tetrabutyl titanate
Orthotitanic acid tetrabutylester
TNBT

Molecular weight : 340.32 g/mol

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

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number	01-2119967423-33-XXXX	H336	
titanium tetraisopropanolate			
CAS-No.	546-68-9	Flam. Liq. 3; Eye Irrit. 2A; STOT SE 3; H226, H319, H336	>= 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	>= 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

Consult a physician. Show this material safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

If swallowed

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

Dry powder Dry sand

Unsuitable extinguishing media

Do NOT use water jet.

5.2 Special hazards arising from the substance or mixture

Carbon oxides
Titanium/titanium oxides
Combustible.

5.3 Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

5.4 Further information

Use water spray to cool unopened containers.

SECTION 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapors accumulating to form explosive concentrations. Vapors can accumulate in low areas.

For personal protection see section 8.

6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

6.3 Methods and materials for containment and cleaning up

Contain spillage, and then collect with non-combustible absorbent material, (e.g. sand, earth, diatomaceous earth, vermiculite) and place in container for disposal according to local / national regulations (see section 13).

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

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist.

Advice on protection against fire and explosion

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

Hygiene measures

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

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. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

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	USA. OSHA - TABLE Z-1 Limits for Air Contaminants - 1910.1000
		Skin notation		
		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

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Tightly fitting safety goggles. Faceshield (8-inch minimum). Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

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: Fluorinated rubber

Minimum layer thickness: 0.7 mm

Break through time: 480 min

Material tested: Vitoject® (KCL 890 / Aldrich Z677698, Size M)

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0.4 mm

Break through time: 240 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, 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

Complete suit protecting against chemicals, Flame retardant antistatic protective clothing., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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 | No data available |
| f) Initial boiling point and boiling range | 206 °C 403 °F at 13 hPa |
| g) Flash point | 50 °C (122 °F) |
| 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 | No data available |
| n) Water solubility | No data available |

- o) Partition coefficient: No data available
n-octanol/water
- p) Autoignition No data available
temperature
- q) Decomposition No data available
temperature
- 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

No data available

10.2 Chemical stability

Stable under recommended storage conditions.

10.3 Possibility of hazardous reactions

No data available

10.4 Conditions to avoid

Heat, flames and sparks.

10.5 Incompatible materials

Strong acids and oxidizing agents

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

No data available

Acute toxicity estimate Oral - 2,893 mg/kg

(Calculation method)

Inhalation: No data available

Acute toxicity estimate Inhalation - 4 h - 155.6 mg/l

(Calculation method)

Dermal: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg

(Calculation method)

No data available

Skin corrosion/irritation

No data available

Serious eye damage/eye irritation

No data available

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

No data available

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

RTECS: XR1585000

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

Ames test
Escherichia coli/Salmonella typhimurium
Result: negative
Chromosome aberration test in vitro
Human lymphocytes
Result: negative
In vitro mammalian cell gene mutation test
mouse lymphoma cells
Result: negative

Carcinogenicity

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

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

Ames test
S. typhimurium
Result: negative
US-EPA
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

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

Mutagenicity (mammal cell test): micronucleus.

Chinese hamster lung cells

Result: negative

Remarks:

(ECHA)

In vitro mammalian cell gene mutation test

Chinese hamster lung cells

Result: negative

OECD Test Guideline 474

Mouse - male and female

Result: negative

Carcinogenicity

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

No data available

Toxicity to daphnia static test EC50 - Daphnia magna (Water flea) - 590 mg/l - 48
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and other aquatic invertebrates	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

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

Offer surplus and non-recyclable solutions to a licensed disposal company. Burn in a chemical incinerator equipped with an afterburner and scrubber but exert extra care in igniting as this material is highly flammable. Contact a licensed professional waste disposal service to dispose of this material.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

DOT (US)

UN number: 1993 Class: 3 Packing group: III
 Proper shipping name: Flammable liquids, n.o.s. (titanium tetraisopropanolate, 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. (titanium tetraisopropanolate, n-butanol)

IATA

UN number: 1993 Class: 3 Packing group: III

Proper shipping name: Flammable liquid, n.o.s. (titanium tetraisopropanolate, 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

The following components are subject to reporting levels established by SARA Title III, Section 313:

	CAS-No.	Revision Date
n-butanol	71-36-3	2007-07-01

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.

Pennsylvania Right To Know Components

	CAS-No.	Revision Date
tetra-n-butyl orthotitanate	5593-70-4	
titanium tetraisopropanolate	546-68-9	

SECTION 16: Other information

Further information

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