



SAFETY DATA SHEET

according to the (US) Hazard Communication Standard (29 CFR 1910.1200)

Revision Date 07/30/2015

Version 2.0

SECTION 1. Identification

Product identifier

Product number	821084
Product name	Tetra-n-butyl orthotitanate for synthesis
CAS-No.	5593-70-4

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

Identified uses	Chemical for synthesis
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Details of the supplier of the safety data sheet

Company	EMD Millipore Corporation 290 Concord Road, Billerica, MA 01821, United States of America General Inquiries: +1-978-715-4321 Monday to Friday, 9:00 AM to 4:00 PM Eastern Time (GMT-5)
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Emergency telephone	800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week
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SECTION 2. Hazards identification

GHS Classification

Flammable liquid, Category 3, H226

Skin irritation, Category 2, H315

Serious eye damage, Category 1, H318

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

GHS-Labeling

Hazard pictograms



Signal Word

Danger

Hazard Statements

H226 Flammable liquid and vapor.

H315 Causes skin irritation.

H318 Causes serious eye damage.

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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.
P264 Wash skin thoroughly after handling.
P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.
P303 + P361 + P353 IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P310 Immediately call a POISON CENTER or doctor/ physician.
P321 Specific treatment (see supplemental first aid instructions on this label).
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 for extinction.
P403 + P235 Store in a well-ventilated place. Keep cool.
P501 Dispose of contents/ container to an approved waste disposal plant.

Other hazards

None known.

SECTION 3. Composition/information on ingredients

Formula	$(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O})_4\text{Ti}$	$\text{C}_{16}\text{H}_{36}\text{O}_4\text{Ti}$ (Hill)
Molar mass	340.32 g/mol	

Hazardous ingredients

Chemical Name (Concentration)

CAS-No.

tetra-n-butyl orthotitanate ($\geq 90\%$ - $\leq 100\%$)

5593-70-4

Exact percentages are being withheld as a trade secret.

titanium tetraisopropanolate ($\geq 1\%$ - $< 5\%$)

546-68-9

Exact percentages are being withheld as a trade secret.

n-butanol ($\geq 1\%$ - $< 5\%$)

71-36-3

Exact percentages are being withheld as a trade secret.

SECTION 4. First aid measures

Description of first-aid measures

Inhalation

After inhalation: fresh air.

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Skin contact

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

Eye contact

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

Ingestion

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

Never give anything by mouth to an unconscious person.

Most important symptoms and effects, both acute and delayed

Irritation and corrosion, Dizziness, Headache, Vertigo

Risk of serious damage to eyes.

Indication of any immediate medical attention and special treatment needed

No information available.

SECTION 5. Fire-fighting measures

Extinguishing media

Suitable extinguishing media

Foam, Carbon dioxide (CO₂), Dry powder

Unsuitable extinguishing media

Water

Special hazards arising from the substance or mixture

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 vapors possible in the event of fire.

Advice for firefighters

Special protective equipment for fire-fighters

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

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

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.

Advice for emergency responders:

Protective equipment see section 8.

Environmental precautions

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Do not let product enter drains. Risk of explosion.

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.

SECTION 7. Handling and storage

Precautions for safe handling

Observe label precautions.

Advice on protection against fire and explosion

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

Conditions for safe storage, including any incompatibilities

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

Store at +2°C to +8°C (+36°F to +46°F).

SECTION 8. Exposure controls/personal protection

Exposure limit(s)

Ingredients

Basis	Value	Threshold limits	Remarks
<i>n-butanol 71-36-3</i>			
ACGIH	Time Weighted Average (TWA):	20 ppm	Can be absorbed through the skin.
NIOSH/GUIDE	Skin designation:		
	Ceiling Limit Value and Time Period (if specified):	50 ppm 150 mg/m ³	
OSHA_TRANS	PEL:	100 ppm 300 mg/m ³	
Z1A	Ceiling Limit Value:	50 ppm 150 mg/m ³	
	Skin designation (Final Rule Limit applies):		Can be absorbed through the skin.

Engineering measures

Technical measures and appropriate working operations should be given priority over the use of personal protective equipment.

Individual protection measures

Protective clothing should be selected specifically for the workplace, depending on concentration and quantity of the hazardous substances handled. The chemical resistance of the protective equipment should be inquired at the respective supplier.

Hygiene measures

Immediately change contaminated clothing. Apply skin- protective barrier cream. Wash hands and face after working with substance.

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Eye/face protection

Tightly fitting safety goggles

Hand protection

full contact:

Glove material: butyl-rubber
Glove thickness: 0.70 mm
Break through time: > 480 min

splash contact:

Glove material: Nitrile rubber
Glove thickness: 0.40 mm
Break through time: > 30 min

The protective gloves to be used must comply with the specifications of EC Directive 89/686/EEC and the related standard EN374, for example KCL 898 Butoject® (full contact), KCL 730 Camatril® - Velours (splash contact).

The breakthrough times stated above were determined by KCL in laboratory tests acc. to EN374 with samples of the recommended glove types.

This recommendation applies only to the product stated in the safety data sheet and supplied by us as well as to the purpose specified by us. 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).

Other protective equipment:

Flame retardant antistatic protective clothing.

Respiratory protection

required when vapors/aerosols are generated.

Recommended Filter type: Filter A-(P2)

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are performed according to the instructions of the producer. These measures have to be properly documented.

SECTION 9. Physical and chemical properties

Physical state	liquid
Color	light yellow
Odor	aromatic
Odor Threshold	No information available.
pH	No information available.
Melting point	-40 °C
Boiling point/boiling range	310 - 314 °C (310 - 314 °C) at 1,013 hPa
Flash point	47 °C (47 °C)

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Evaporation rate	No information available.
Flammability (solid, gas)	No information available.
Lower explosion limit	2.0 %(V)
Upper explosion limit	12.0 %(V)
Vapor pressure	5.6 hPa at 20 °C (20 °C)
Relative vapor density	No information available.
Density	0.99 g/cm ³ at 20 °C (20 °C)
Relative density	No information available.
Water solubility	at 20 °C (20 °C) (slow decomposition)
Partition coefficient: n-octanol/water	No information available.
Autoignition temperature	No information available.
Decomposition temperature	No information available.
Viscosity, dynamic	90 mPa.s at 20 °C (20 °C)
Explosive properties	No information available.
Oxidizing properties	none

SECTION 10. Stability and reactivity

Reactivity

Vapor/air-mixtures are explosive at intense warming.

Chemical stability

sensitive to moisture

Possibility of hazardous reactions

Exothermic reaction with:

Water

Violent reactions possible with:

Strong oxidizing agents, alkalines

Conditions to avoid

Heating.

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Exposure to moisture.

Incompatible materials

no information available

Hazardous decomposition products

no information available

SECTION 11. Toxicological information

Information on toxicological effects

Likely route of exposure

Inhalation, Eye contact, Skin contact

Target Organs

Eyes

Skin

Respiratory system

Central nervous system

Acute oral toxicity

LD50 Rat: 3,122 mg/kg (RTECS)

Symptoms: Risk of aspiration upon vomiting., Aspiration may cause pulmonary edema and pneumonitis.

Acute inhalation toxicity

LC50 Rat: 11 mg/l; 4 h ; dust/mist

Symptoms: Possible damages:, mucosal irritations
(External MSDS)

Skin irritation

Causes skin irritation.

Eye irritation

Causes serious eye damage.

Risk of blindness!

Specific target organ systemic toxicity - single exposure

The substance or mixture is not classified as specific target organ toxicant, single exposure.

Specific target organ systemic toxicity - repeated exposure

The substance or mixture is not classified as specific target organ toxicant, repeated exposure.

Aspiration hazard

Regarding the available data the classification criteria are not fulfilled.

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.

OSHA

No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by OSHA.

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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.

ACGIH No ingredient of this product present at levels greater than or equal to 0.1% is identified as a carcinogen or potential carcinogen by ACGIH.

Further information

After absorption:

Irritation and corrosion, Headache, Dizziness, Vertigo

Risk of blindness!

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

Ingredients

tetra-n-butyl orthotitanate

Eye irritation

Rabbit

Result: Eye irritation

titanium tetraisopropanolate

Acute oral toxicity

LD50 Rat: 7,500 mg/kg (External MSDS)

Acute inhalation toxicity

LC50 Rat: 7.78 mg/l; 4 h ; aerosol Aerosol (External MSDS)

Acute dermal toxicity

LD50 Rabbit: > 15,200 mg/kg (RTECS)

Skin irritation

Rabbit

Result: slight irritation
(External MSDS)

Eye irritation

Rabbit

Result: Eye irritation
(External MSDS)

n-butanol

Acute oral toxicity

LD50 Rat: 790 mg/kg (RTECS)

Acute dermal toxicity

LD50 Rabbit: 3,400 mg/kg (RTECS)

Skin irritation

Rabbit

Result: Irritations
(IUCRID)

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Eye irritation

Rabbit

Result: Severe irritations

OECD Test Guideline 405

Germ cell mutagenicity

Genotoxicity in vitro

Ames test

Salmonella typhimurium

Result: negative

(IUCLID)

SECTION 12. Ecological information

Ecotoxicity

No information available.

Persistence and degradability

No information available.

Bioaccumulative potential

No information available.

Mobility in soil

No information available.

Additional ecological information

Discharge into the environment must be avoided.

Ingredients

tetra-n-butyl orthotitanate

No information available.

titanium tetraisopropanolate

No information available.

n-butanol

Toxicity to fish

LC50 *Leuciscus idus* (Golden orfe): 1,200 - 1,700 mg/l; 96 h (IUCLID)

Toxicity to daphnia and other aquatic invertebrates

EC50 *Daphnia magna* (Water flea): 1,983 mg/l; 48 h

DIN 38412

Toxicity to algae

IC50 *Desmodesmus subspicatus* (green algae): > 500 mg/l; 72 h (IUCLID)

Toxicity to bacteria

EC10 *Pseudomonas putida*: 2,250 mg/l; 16 h (IUCLID)

Biodegradability

98 %; 28 d

OECD Test Guideline 301E

Readily biodegradable.

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Ratio BOD/ThBOD
BOD5 33 %
(IUCLID)

Substance does not meet the criteria for PBT or vPvB according to Regulation (EC) No 1907/2006, Annex XIII.

SECTION 13. Disposal considerations

The information presented only applies to the material as supplied. The identification based on characteristic(s) or listing may not apply if the material has been used or otherwise contaminated. It is the responsibility of the waste generator to determine the toxicity and physical properties of the material generated to determine the proper waste identification and disposal methods in compliance with applicable regulations. Disposal should be in accordance with applicable regional, national and local laws and regulations.

SECTION 14. Transport information

Land transport (DOT)

UN number UN 1993
Proper shipping name FLAMMABLE LIQUID, N.O.S.
(TETRABUTYLORTHOTITANATE)
Class 3
Packing group III
Environmentally hazardous --

Air transport (IATA)

UN number UN 1993
Proper shipping name FLAMMABLE LIQUID, N.O.S.
(TETRABUTYLORTHOTITANATE)
Class 3
Packing group III
Environmentally hazardous --
Special precautions for user no

Sea transport (IMDG)

UN number UN 1993
Proper shipping name FLAMMABLE LIQUID, N.O.S.
(TETRABUTYLORTHOTITANATE)
Class 3
Packing group III
Environmentally hazardous --
Special precautions for user yes
EmS F-E S-E

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SECTION 15. Regulatory information

United States of America

SARA 313

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

Ingredients

n-butanol	71-36-3	2.4999 %
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SARA 302

No chemicals in this material are subject to the reporting requirements of SARA Title III, Section 302.

Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. CleanWater Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

DEA List I

Not listed

DEA List II

Not listed

US State Regulations

Massachusetts Right To Know

Ingredients

n-butanol

Pennsylvania Right To Know

Ingredients

n-butanol

New Jersey Right To Know

Ingredients

n-butanol

California Prop 65 Components

This product does not contain any chemicals known to the State of California to cause cancer, birth, or any other reproductive defects.

Notification status

TSCA: All components of the product are listed in the TSCA-inventory.

DSL: All components of this product are on the Canadian DSL.

SECTION 16. Other information

Training advice

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Provide adequate information, instruction and training for operators.

Labeling

Hazard pictograms



Signal Word

Danger

Hazard Statements

H226 Flammable liquid and vapor.

H315 Causes skin irritation.

H318 Causes serious eye damage.

Precautionary Statements

Prevention

P210 Keep away from heat.

P280 Wear eye protection.

Response

P302 + P352 IF ON SKIN: Wash with plenty of soap and water.

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

P313 Get medical advice/ attention.

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

H226 Flammable liquid and vapor.

H315 Causes skin irritation.

H318 Causes serious eye damage.

Key or legend to abbreviations and acronyms used in the safety data sheet

Used abbreviations and acronyms can be looked up at www.wikipedia.org.

Revision Date 07/30/2015

The information contained herein is based on the present state of our knowledge. It characterizes the product with regard to appropriate safety precautions. It does not represent a warranty of any product properties and we assume no liability for any loss or injury which may result from the use of this information. Users should conduct their own investigations to determine the suitability of the information.

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