

# SAFETY DATA SHEET

Version 6.14  
Revision Date 09/06/2024  
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## 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

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 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 Statements

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 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 mist or vapors.
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

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### SECTION 3: Composition/information on ingredients

#### 3.2 Mixtures

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The life science business of Merck KGaA, Darmstadt, Germany operates as MilliporeSigma in the US and Canada

**MILLIPORE  
SIGMA**

Formula : C<sub>16</sub>H<sub>36</sub>O<sub>4</sub>Ti  
Molecular weight : 340.32 g/mol

Component		Classification	Concentration
<b>tetra-n-butyl orthotitanate</b>			
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		
<b>titanium tetraisopropanolate</b>			
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		
<b>n-butanol</b>			
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;	>= 1 - < 5 %
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

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

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### **SECTION 5: Firefighting measures**

#### **5.1 Extinguishing media**

##### **Suitable extinguishing media**

Water Foam Carbon dioxide (CO<sub>2</sub>) 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.

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.

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### **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.

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## 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

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

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## 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 <sup>3</sup>	USA. NIOSH Recommended Exposure Limits
	Remarks	Potential for dermal absorption		
		TWA	100 ppm 300 mg/m <sup>3</sup>	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
		C	50 ppm 150 mg/m <sup>3</sup>	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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://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 EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://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

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.

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## 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) Density	1.00 g/mL at 20 °C (68 °F) - lit.
Relative density	0.9925 °C
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

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## 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

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## 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

Remarks: Mixture causes skin irritation.

#### Serious eye damage/eye irritation

Remarks: 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**

**tetra-n-butyl orthotitanate**

**Acute toxicity**

LD50 Oral - Rat - 3,122 mg/kg

Remarks: (RTECS)

Inhalation: No data available

Dermal: No data available

**Skin corrosion/irritation**

Remarks: Causes skin irritation.

(ECHA)

**Serious eye damage/eye irritation**

Remarks: 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)

**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

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**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 Endocrine disrupting properties**

No data available

**12.7 Other adverse effects**

No data available

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## Components

### tetra-n-butyl orthotitanate

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

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)

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## 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.

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**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  
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)

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**SECTION 15: Regulatory information****CERCLA Reportable Quantity**

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
n-butanol	71-36-3	100	100 (F003)

**SARA 304 Extremely Hazardous Substances Reportable Quantity**

This material does not contain any components with a section 304 EHS RQ.

**SARA 302 Extremely Hazardous Substances Threshold Planning Quantity**

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

**SARA 311/312 Hazards** : Fire Hazard  
Acute Health Hazard  
Chronic Health Hazard

**SARA 313** : The following components are subject to reporting levels established by SARA Title III, Section 313:  
n-butanol 71-36-3 >= 1 - < 5 %

**Clean Air Act**

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).  
This product does not contain any hazardous air pollutants (HAP), as defined by the U.S. Clean Air Act Section 112 (40 CFR 61).  
This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).  
The following chemical(s) are listed under the U.S. Clean Air Act Section 111 SOCM I Intermediate or Final VOC's (40 CFR 60.489):

n-butanol

71-36-3

>= 1 - < 5 %

### **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

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

n-butanol

71-36-3

#### **Pennsylvania Right To Know**

n-butanol

71-36-3

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

### **The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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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 Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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