• SAFETY DATA SHEET

Version 6.16
Revision Date 11/06/2025
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SECTION 1. IDENTIFICATION

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

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 number

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Flammable liquids : Category 3

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Skin irritation	:	Category 2
Serious eye damage	:	Category 1
Specific target organ toxicity - single exposure	:	Category 3 (Respiratory system, Central nervous system)

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Danger

Hazard statements :
H226 Flammable liquid and vapour.
H315 Causes skin irritation.
H318 Causes serious eye damage.
H335 May cause respiratory irritation.
H336 May cause drowsiness or dizziness.

Precautionary statements :

Prevention:

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 vapours.
P264 Wash skin thoroughly after handling.
P271 Use only outdoors or in a well-ventilated area.
P280 Wear protective gloves/ eye protection/ face protection.

Response:

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.

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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.

Storage:

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.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 5593-70-4

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
tetra-n-butyl orthotitanate	5593-70-4*	>= 90 - <= 100	-
titanium tetraisopropanolate	546-68-9*	>= 5 - < 10	-
n-butanol	71-36-3*	>= 1 - < 5	-

* Indicates that the identifier is a CAS No.
Actual concentration is withheld as a trade secret

SECTION 4. FIRST AID MEASURES

General advice : Show this 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.

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If swallowed	:	After swallowing: immediately make victim drink water (two glasses at most). Consult a physician.
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
Protection of first-aiders	:	For personal protection see section 8.
Notes to physician	:	No data available

SECTION 5. FIREFIGHTING MEASURES

Suitable extinguishing media	:	Water Foam Carbon dioxide (CO2) Dry powder
Unsuitable extinguishing media	:	For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	:	Combustible. Vapours 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.
Hazardous combustion products	:	Carbon oxides Titanium/titanium oxides
Specific extinguishing methods	:	No data available
Further information	:	Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating

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surface water or the ground water system.

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.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	:	Advice for non-emergency personnel: Do not breathe vapours, 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: For personal protection see section 8.
Environmental precautions	:	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

For precautions see section 2.2.

Advice on protection against fire and explosion	:	Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.
Advice on safe handling	:	Work under hood. Do not inhale substance/mixture. Avoid generation of vapours/aerosols.
Further information on storage conditions	:	Keep container tightly closed in a dry and well-ventilated place. Keep away from heat and sources of ignition.
Storage class	:	3, Flammable liquids
Recommended storage temperature	:	Recommended storage temperature see product label.

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Further information on storage stability : Air and moisture sensitive.

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentration	Basis
n-butanol	71-36-3	TWA	20 ppm	ACGIH
		C	50 ppm 150 mg/m3	NIOSH REL
		TWA	100 ppm 300 mg/m3	OSHA Z-1
		TWA	2 ppm	US WEEL
		STEL	5 ppm	US WEEL

Engineering measures : No data available

Personal protective equipment

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.

Recommended Filter type: : Filter type ABEK

The entrepeneur 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.

Hand protection

Material	:	butyl-rubber
Break through time	:	480 min
Glove thickness	:	0.7 mm
Protective index	:	Full contact
Manufacturer	:	KCL 898 Butoject®
Material	:	Nitrile rubber
Break through time	:	30 min
Glove thickness	:	0.4 mm

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Protective index	:	Splash contact
Manufacturer	:	Camatril® (KCL 730 / Aldrich Z677442, Size M)
Remarks	:	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).
Eye 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 and body protection	:	Flame retardant antistatic protective clothing.
Hygiene measures	:	Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	:	liquid
Color	:	light yellow
Odor	:	No data available
Odor Threshold	:	No data available
pH	:	No data available
Melting point/ range	:	< -103 °F / < -75 °C Decomposition: yes Method: OECD Test Guideline 102 GLP: yes
Boiling point/boiling range	:	403 °F / 206 °C (13 hPa)
Flash point	:	108 °F / 42 °C Method: ASTM D 93, Pensky-Martens closed cup
Evaporation rate	:	No data available
Flammability (solid, gas)	:	No data available

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Flammability (liquids)	:	No data available
Burning rate	:	No data available
Upper explosion limit / Upper flammability limit	:	No data available
Lower explosion limit / Lower flammability limit	:	No data available
Vapor pressure	:	No data available
Relative vapour density	:	No data available
Relative density	:	0.99 (77 °F / 25 °C)
Density	:	1.00 g/mL (68 °F / 20 °C)
Water solubility	:	No data available
Partition coefficient: n-octanol/water	:	No data available
Autoignition temperature	:	No data available
Decomposition temperature	:	No data available
Viscosity		
Viscosity, dynamic	:	ca. 66 mPa.s (77 °F / 25 °C)
Viscosity, kinematic	:	No data available
Flow time	:	No data available
Explosive properties	:	Not classified as explosive.
Oxidizing properties	:	none
Refractive index	:	1.491
Molecular weight	:	340.32 g/mol
Particle characteristics		
Particle size	:	No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	:	Vapour/air-mixtures are explosive at intense warming.

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Chemical stability	:	The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	:	No data available
Conditions to avoid	:	Heating.
Incompatible materials	:	Strong acids and oxidizing agents Water
Hazardous decomposition products	:	In the event of fire: see section 5

SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity
Oral: No data available
Acute toxicity estimate Oral - 2,893 mg/kg
(Calculation method)
LD50 Oral - Rat - 3,122 mg/kg
Remarks: (RTECS)

Inhalation: No data available

Dermal: No data available

Acute toxicity estimate Dermal - > 5,000 mg/kg
(Calculation method)

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
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 471
Result: negative
Test Type: Chromosome aberration test in vitro
Test system: Human lymphocytes
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 473
Result: negative

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Test Type: In vitro mammalian cell gene mutation test
Test system: mouse lymphoma cells
Metabolic activation: with and without metabolic activation
Method: OECD Test Guideline 476
Result: negative

Carcinogenicity

IARC: No component 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 component 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
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

11.2 Additional Information

RTECS: XR1585000
To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

titanium tetraisopropanolate:

Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 590 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes

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Toxicity to algae/aquatic plants	:	ErC50 (Desmodesmus subspicatus (green algae)): > 820 mg/l Exposure time: 72 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
Toxicity to microorganisms	:	EC50 (Bacteria): 1,050 mg/l Exposure time: 16 h

n-butanol:

Toxicity to fish	:	LC50 (Pimephales promelas (fathead minnow)): 1,376 mg/l End point: mortality Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 203 GLP: yes
Toxicity to daphnia and other aquatic invertebrates	:	EC50 (Daphnia magna (Water flea)): 1,328 mg/l End point: Immobilization Exposure time: 48 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 202 GLP: yes
Toxicity to algae/aquatic plants	:	ErC50 (Pseudokirchneriella subcapitata (green algae)): 225 mg/l Exposure time: 96 h Test Type: static test Analytical monitoring: yes Method: OECD Test Guideline 201 GLP: yes
Toxicity to daphnia and other aquatic invertebrates (Chronic toxicity)	:	EC50 (Daphnia magna (Water flea)): 18 mg/l End point: reproduction rate Exposure time: 21 d Test Type: semi-static test Analytical monitoring: yes Method: OECD Test Guideline 211 GLP: yes
Toxicity to microorganisms	:	EC50 (Pseudomonas putida): 4,390 mg/l Exposure time: 17 h Test Type: static test Method: DIN 38421 TEIL 8

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Persistence and degradability

Components:

n-butanol:

Biodegradability	:	aerobic Concentration: 3 mg/l Result: Readily biodegradable. Biodegradation: 92 % Exposure time: 20 d Remarks: (ECHA)
BOD/ThOD	:	33 % Remarks: (IUCLID)

Bioaccumulative potential

Components:

n-butanol:

Bioaccumulation	:	Species: Oncorhynchus mykiss (rainbow trout) Bioconcentration factor (BCF): 0.38 Exposure time: 24 h Concentration: 921 mg/l
Partition coefficient: n-octanol/water	:	log Pow: 1 (77 °F / 25 °C) pH: 7 Method: OECD Test Guideline 117 GLP: yes Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

Product:

Ozone-Depletion Potential	:	Regulation: 40 CFR Protection of Environment; Part 82 Protection of Stratospheric Ozone - CAA Section 602 Class I Substances Remarks: 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).

Components:

titanium tetraisopropanolate:

Additional ecological information	:	Discharge into the environment must be avoided.

n-butanol:

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

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues	:	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.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

UN/ID No.	:	UN 1993
Proper shipping name	:	Flammable liquid, n.o.s. (titanium tetraisopropanolate, n-butanol)
Class	:	3
Packing group	:	III
Labels	:	Class 3 - Flammable liquids
Packing instruction (cargo aircraft)	:	366
Packing instruction (passenger aircraft)	:	355

IMDG-Code

UN number	:	UN 1993
Proper shipping name	:	FLAMMABLE LIQUID, N.O.S. (titanium tetraisopropanolate, n-butanol)
Class	:	3
Packing group	:	III
Labels	:	3
EmS Code	:	F-E, S-E
Marine pollutant	:	no

Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR Road

UN/ID/NA number	:	UN 1993
Proper shipping name	:	Flammable liquids, n.o.s. (titanium tetraisopropanolate, n-butanol)
Class	:	3
Packing group	:	III
Labels	:	Class 3 - Flammable liquids
ERG Code	:	128

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Marine pollutant : no

Poison Inhalation Hazard : No

Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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 SOCMI 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

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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 components 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.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

ACGIH	:	USA. ACGIH Threshold Limit Values (TLV)
NIOSH REL	:	USA. NIOSH Recommended Exposure Limits
OSHA Z-1	:	USA. Occupational Exposure Limits (OSHA) - Table Z-1 Limits for Air Contaminants
US WEEL	:	USA. Workplace Environmental Exposure Levels (WEEL)
ACGIH / TWA	:	8-hour, time-weighted average
NIOSH REL / C	:	Ceiling value not be exceeded at any time.
OSHA Z-1 / TWA	:	8-hour time weighted average
US WEEL / TWA	:	8-hr TWA
US WEEL / STEL	:	Short-Term TWA

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and

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Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.
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Revision Date : 11/06/2025

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US / EN

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