

SAFETY DATA SHEET

Version 6.6 Revision Date 12/23/2020 Print Date 02/05/2022

SECTION 1: Identification of the substance/mixture and of the company/undertaking

1.1 Product identifiers

1.2

2	Relevant identified use	es	of the substance or mixture and uses advised against
	Product Number Brand	-	416665 Aldrich
	Product name	:	tert-Butyl hydroperoxide solution

Identified uses : Laboratory chemicals, Synthesis of substances

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 Fax		+1 314 771-5765 +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 Organic peroxides (Type D), H242 Acute toxicity, Oral (Category 4), H302 Acute toxicity, Inhalation (Category 3), H331 Acute toxicity, Dermal (Category 3), H311 Skin corrosion (Category 1C), H314 Serious eye damage (Category 1), H318 Skin sensitization (Category 1), H317 Germ cell mutagenicity (Category 2), H341 Aspiration hazard (Category 1), H304 Short-term (acute) aquatic hazard (Category 2), H401 Long-term (chronic) aquatic hazard (Category 2), H411

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

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2.2 GHS Label elements, including precautionary statements

Pictogram	
Signal word	Danger
Hazard statement(s) H226 H242 H302	Flammable liquid and vapor. Heating may cause a fire. Harmful if swallowed.
H304	May be fatal if swallowed and enters airways.
H311 + H331	Toxic in contact with skin or if inhaled.
H314 H317	Causes severe skin burns and eye damage. May cause an allergic skin reaction.
H317 H341	Suspected of causing genetic defects.
H411	Toxic to aquatic life with long lasting effects.
Precautionary statement(s)	
P201 , , , , , , , , , , , , , , , , , , ,	Obtain special instructions before use.
P202	Do not handle until all safety precautions have been read and understood.
P210	Keep away from heat/ sparks/ open flames/ hot surfaces. No smoking.
P220	Keep/Store away from clothing/ combustible materials.
P233	Keep container tightly closed.
P234	Keep only in original container.
P240	Ground/bond container and receiving equipment.
P241	Use explosion-proof electrical/ventilating/lighting/ equipment.
P242	Use only non-sparking tools.
P243 P261	Take precautionary measures against static discharge. Avoid breathing dust/ fume/ gas/ mist/ vapors/ spray.
P264	Wash skin thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P271	Use only outdoors or in a well-ventilated area.
P272	Contaminated work clothing should not be allowed out of the workplace.
P273	Avoid release to the environment.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P235	Keep cool.
P301 + P310	IF SWALLOWED: Immediately call a POISON CENTER/ doctor.
P301 + P330 + P331	IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.
P303 + P361 + P353	IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower.
P304 + P340	IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing.
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/ doctor.
P322	Specific measures (see supplemental first aid instructions on this label).
P333 + P313	If skin irritation or rash occurs: Get medical advice/ attention.
P361	Remove/ Take off immediately all contaminated clothing.
P363	Wash contaminated clothing before reuse.

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P370 + P378	In case of fire: Use dry sand, dry chemical or alcohol-resistant foam for extinction.
P391	Collect spillage.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
P405	Store locked up.
P410	Protect from sunlight.
P420	Store away from other materials.
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

	• •	5		
3.2	Mixtures Synonyms	: TBHP		
	Formula	: $C_4H_{10}O_2$		
	Molecular weight	: 90.12 g/mol		
	Component		Classification	Concentration
	decane			
	CAS-No. EC-No.	124-18-5 204-686-4	Flam. Liq. 3; Asp. Tox. 1; H226, H304	>= 50 - < 70 %
	tert-Butyl hydropero>	cide		
	CAS-No. EC-No.	75-91-2 200-915-7	Flam. Liq. 3; Org. Perox. A; Acute Tox. 4; Acute Tox. 3; Skin Corr. 1C; Eye Dam. 1; Muta. 2; Aquatic Acute 2; Aquatic Chronic 2; H226, H240, H302, H332, H311, H314, H318, H341, H401, H411	>= 50 - < 70 %

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

First aider needs to protect himself. 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. Call a physician immediately.

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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: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Pulmonary failure possible after aspiration of vomit. Call a physician immediately. Do not attempt to neutralise.

- **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

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

Mixture with combustible ingredients. 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.

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 carefully with liquid-absorbent material (e.g. Chemizorb®). Dispose of properly. Clean up affected area.

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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 locked up or in an area accessible only to qualified or authorized persons. Separately or together with other organic peroxides only and away from sources of ignition and heat.

Storage stability

Recommended storage temperature 2 - 8 °C

Storage class (TRGS 510): 5.2: Organic peroxides and self-reacting hazardous materials

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
tert-Butyl hydroperoxide	75-91-2	TWA	0.1 ppm	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Danger of cutaneous absorption		

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

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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: Nitrile rubber Minimum layer thickness: 0.4 mm Break through time: 480 min Material tested:Camatril® (KCL 730 / Aldrich Z677442, Size M)

Splash contact Material: Nitrile rubber Minimum layer thickness: 0.2 mm Break through time: 60 min Material tested:Dermatril® P (KCL 743 / Aldrich Z677388, 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

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
b)	Odor	No data available
c)	Odor Threshold	No data available
d)	рН	No data available
e)	Melting point/freezing point	No data available
f)	Initial boiling point and boiling range	No data available
g)	Flash point	43 °C (109 °F) - closed cup
h)	Evaporation rate	No data available

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i)	Flammability (solid,	No data available
	gas)	

j)	Upper/lower	No data available
	flammability or	
	explosive limits	

- k) Vapor pressure No data available
- I) Vapor density No data available
- m) Relative density 0.808 g/cm³
- 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

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** Powdered metals, Strong oxidizing agents, Organic materials
- **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

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Inhalation: No data available

Acute toxicity estimate Inhalation - 4 h - 3.42 mg/l (Calculation method) Symptoms: mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract Dermal: No data available

Acute toxicity estimate Dermal - 813.73 mg/kg (Calculation method) No data available

Skin corrosion/irritation

Mixture causes burns.

Serious eye damage/eye irritation

Mixture causes serious eye damage. Risk of blindness!

Respiratory or skin sensitization

Mixture may cause an allergic skin reaction.

Germ cell mutagenicity

Evidence of genetic defects.

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

Specific target organ toxicity - single exposure

No data available

Acute inhalation toxicity - mucosal irritations, Cough, Shortness of breath, Possible damages:, damage of respiratory tract

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

Aspiration hazard, Aspiration may cause pulmonary edema and pneumonitis.

11.2 Additional Information

Not available

Material is extremely destructive to tissue of the mucous membranes and upper respiratory tract, eyes, and skin., spasm, inflammation and edema of the larynx, spasm, inflammation and edema of the bronchi, pneumonitis, pulmonary edema, burning sensation, Cough, wheezing, laryngitis, Shortness of breath, Headache, Nausea

Other dangerous properties can not be excluded.

This substance should be handled with particular care.

Handle in accordance with good industrial hygiene and safety practice.

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Stomach - Irregularities - Based on Human Evidence

Components

decane

Acute toxicity

LD50 Oral - Rat - male and female - > 5,000 mg/kg (OECD Test Guideline 401) LC50 Inhalation - Rat - male - 8 h - > 1369 ppm (OECD Test Guideline 403) LC50 Inhalation - Rat - male and female - 4 h - > 5.6 mg/l (OECD Test Guideline 403) LD50 Dermal - Rabbit - male and female - > 5,000 mg/kg (OECD Test Guideline 402) No data available

Skin corrosion/irritation

Skin - Rabbit Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit Result: No eye irritation (OECD Test Guideline 405)

Respiratory or skin sensitization

Maximization Test - Guinea pig Result: Does not cause skin sensitization. (OECD Test Guideline 406)

Germ cell mutagenicity

Ames test S. typhimurium Result: negative Mutagenicity (micronucleus test) Mouse - male and female Result: negative

Carcinogenicity

Reproductive toxicity

No data available 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

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tert-Butyl hydroperoxide

Acute toxicity

LD50 Oral - Rat - male and female - 560 mg/kg Remarks: Aqueous solution (ECHA) LC50 Inhalation - Rat - male and female - 4 h - 1.85 mg/l (OECD Test Guideline 403) Remarks: (in analogy to similar products) LD50 Dermal - Rabbit - male and female - 440 mg/kg (OECD Test Guideline 402) Remarks: Aqueous solution No data available

Skin corrosion/irritation

Skin - Rabbit Result: Corrosive, category 1C - where responses occur after exposures between 1 hour and 4 hours and observations up to 14 days. - 24 h Remarks: Aqueous solution

Serious eye damage/eye irritation

Eyes - Rabbit Result: Corrosive - 21 d Remarks: Aqueous solution

Respiratory or skin sensitization

Maximization Test - Guinea pig Result: positive (OECD Test Guideline 406) Remarks: Aqueous solution

Germ cell mutagenicity

Suspected of causing genetic defects. Mutagenicity (mammal cell test): chromosome aberration. Chinese hamster cells Result: positive Remarks: (in analogy to similar products) In vitro mammalian cell gene mutation test Mouse lymphoma test Result: positive Remarks: (in analogy to similar products) Ames test S. typhimurium Result: positive Remarks: (in analogy to similar products) Regulation (EC) No. 440/2008, Annex, B.12 Mouse - male and female

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Result: negative Remarks: (in analogy to similar products) Regulation (EC) No. 440/2008, Annex, B.12 Mouse - male Result: positive Remarks: (in analogy to similar products)

Rat - male Result: negative Remarks: (in analogy to similar products) (ECHA)

Carcinogenicity

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

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

decane

Toxicity to fish

semi-static test LC50 - Oncorhynchus mykiss (rainbow trout) - > 1,000 mg/l - 96 h (OECD Test Guideline 203)

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Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - > 1,000 mg/l - 48 h
Toxicity to algae	static test EC50 - Pseudokirchneriella subcapitata - > 1,000 mg/l - 72 h (OECD Test Guideline 201)

tert-Butyl hydroperoxide

Toxicity to fish	semi-static test LC50 - Pimephales promelas (fathead minnow) - 29.61 mg/l - 96 h (OECD Test Guideline 203) Remarks: Aqueous solution
Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 14.1 mg/l - 48 h (OECD Test Guideline 202) Remarks: Aqueous solution
Toxicity to algae	static test ErC50 - Pseudokirchneriella subcapitata - 1.5 mg/l - 72 h (OECD Test Guideline 201) Remarks: Aqueous solution
Toxicity to bacteria	Growth inhibition EC50 - activated sludge - 17 mg/l - 30 h (OECD Test Guideline 209) Remarks: Aqueous solution

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Waste material must be disposed of in accordance with the national and loc No mixing with other waste. Handle uncleaned containers like the product 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: 3105 Class: 5.2 (8) Proper shipping name: Organic peroxide type D, liquid (tert-Butyl hydroperoxide, ≤80%) Reportable Quantity (RQ): Poison Inhalation Hazard: No

IMDG

UN number: 3105 Class: 5.2 (8) EMS-No: F-J, S-R Proper shipping name: ORGANIC PEROXIDE TYPE D, LIQUID (tert-BUTYL HYDROPEROXIDE) Aldrich - 416665

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IATA UN number: 3105 Class: 5.2 (8, HEAT) Proper shipping name: Organic peroxide type D, liquid (tert-Butyl hydroperoxide) Special Provisions: "Keep away from heat" label required.

SECTION 15: Regulatory information

SARA 302 Components

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

SARA 313 Components

This material does not contain any chemical components with known CAS numbers that exceed the threshold (De Minimis) reporting levels established by SARA Title III, Section 313.

SARA 311/312 Hazards

Fire Hazard, Reactivity Hazard, Acute Health Hazard, Chronic Health Hazard

Massachusetts Right To Know Components CAS-No. Revision Date

	CAS NO.	Revision Date
tert-Butyl hydroperoxide	75-91-2	2014-05-05

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

Pennsylvania Right To Know Components decane	CAS-No. 124-18-5	Revision Date 2007-03-01
tert-Butyl hydroperoxide	75-91-2	2014-05-05
New Jersey Right To Know Components decane	CAS-No. 124-18-5	Revision Date 2007-03-01
tert-Butyl hydroperoxide	75-91-2	2014-05-05

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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.

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