

SAFETY DATA SHEET

Version 6.3 Revision Date 01/21/2020 Print Date 09/24/2021

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

1.1 Product identifiers

Product name

¹ 2,6-Di(*tert*-butyl-d9)-4-methyl(phenol-3,5,0d3

Product Number	:	452505
Brand	:	Aldrich
CAS-No.	:	64502-99-4

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 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 number

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)

Short-term (acute) aquatic hazard (Category 1), H400 Long-term (chronic) aquatic hazard (Category 1), H410

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

Warning

Aldrich - 452505

Page 1 of 9



Hazard statement(s) H410	Very toxic to aquatic life with long lasting effects.
Precautionary statement(s) P273	Avoid release to the environment.
P391	Collect spillage.
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

Substances Synonyms	: BHT-d21
Formula	: C ₁₅ D ₂₁ H ₃ O
Molecular weight	: 241.06 g/mol
CAS-No.	: 64502-99-4

Component	Classification	Concentration		
2,6-Di(<i>tert-butyl-d<sb>9)-4-methyl(phenol-3,5,<i>O- d<sb>3)</sb></i></sb></i>				
	Aquatic Acute 1; Aquatic Chronic 1; H400, H410 M-Factor - Aquatic Acute: 1 - Aquatic Chronic: 1	<= 100 %		

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 safety data sheet to the doctor in attendance. Move out of dangerous area.

If inhaled

3.1

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

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Aldrich - 452505

Page 2 of 9



- **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 Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

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 Combustible.
- **5.3** Advice for firefighters Wear self-contained breathing apparatus for firefighting if necessary.
- 5.4 Further information No data available

SECTION 6: Accidental release measures

- **6.1 Personal precautions, protective equipment and emergency procedures** Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. 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. Discharge into the environment must be avoided.
- **6.3 Methods and materials for containment and cleaning up** Pick up and arrange disposal without creating dust. Sweep up and shovel. Keep in suitable, closed containers for disposal.
- **6.4** Reference to other sections For disposal see section 13.

SECTION 7: Handling and storage

7.1 Precautions for safe handling

Further processing of solid materials may result in the formation of combustible dusts. The potential for combustible dust formation should be taken into consideration before additional processing occurs.

Provide appropriate exhaust ventilation at places where dust is formed. For precautions see section 2.2.

7.2 Conditions for safe storage, including any incompatibilities Keep container tightly closed in a dry and well-ventilated place.

Aldrich - 452505

Page 3 of 9



Store under inert gas. hygroscopic Storage class (TRGS 510): 11: Combustible Solids

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

Components with workplace control parameters

Component	CAS-No.	Value	Control parameters	Basis
2,6-Di(tert-butyl- d9)-4- methyl(phenol- 3,5,O-d3)	64502-99- 4	TWA	2 mg/m3	USA. ACGIH Threshold Limit Values (TLV)
	Remarks	Upper Respiratory Tract irritation Not classifiable as a human carcinogen		
		TWA	10 mg/m3	USA. NIOSH Recommended Exposure Limits
		PEL	10 mg/m3	California permissible exposure limits for chemical contaminants (Title 8, Article 107)

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

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.

Body Protection

Choose body protection in relation to its type, to the concentration and amount of dangerous substances, and to the specific work-place., The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Respiratory protection is not required. Where protection from nuisance levels of dusts are desired, use type N95 (US) or type P1 (EN 143) dust masks. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Aldrich - 452505

Page 4 of 9



Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

SECTION 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

	-			
a)	Appearance	Form: solid		
b)	Odour	No data available		
c)	Odour Threshold	No data available		
d)	рН	No data available		
e)	Melting point/freezing point	Melting point/range: 69 - 71 °C (156 - 160 °F) - lit.		
f)	Initial boiling point and boiling range	265 °C 509 °F - lit.		
g)	Flash point	127.00 °C (260.60 °F) - closed cup		
h)	Evaporation rate	No data available		
i)	Flammability (solid, gas)	No data available		
j)	Upper/lower flammability or explosive limits	No data available		
k)	Vapour pressure	0.01 hPa at 20.00 °C (68.00 °F)		
I)	Vapour density	No data available		
m)	Relative density	No data available		
n)	Water solubility	No data available		
0)	Partition coefficient: n-octanol/water	No data available		
p)	Auto-ignition temperature	No data available		
q)	Decomposition temperature	No data available		
r)	Viscosity	No data available		
s)	Explosive properties	No data available		
t)	Oxidizing properties	No data available		
Other safety information No data available				

SECTION 10: Stability and reactivity

10.1 Reactivity

No data available

Aldrich - 452505

9.2

Page 5 of 9



10.2 Chemical stability

Stable under recommended storage conditions.

- 10.3 Possibility of hazardous reactions No data available
- **10.4 Conditions to avoid** No data available
- **10.5 Incompatible materials** Acid chlorides, Acid anhydrides, Oxidizing agents, Bases, Brass, Copper, Mild steel, copper compounds
- **10.6 Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - > 6,000 mg/kg (OECD Test Guideline 401) Inhalation: No data available LD50 Dermal - Rat - male and female - > 2,000 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 sensitisation

Patch test: - In vitro study Result: negative Remarks: (ECHA)

Germ cell mutagenicity

In vitro mammalian cell gene mutation test rat hepatocytes Result: negative (ECHA) Ames test Salmonella typhimurium Result: negative (ECHA) Mutagenicity (mammal cell test): chromosome aberration. Chinese hamster ovary cells Result: negative (ECHA)

Aldrich - 452505

Page 6 of 9



Rat - male - Bone marrow Result: negative (ECHA)

Mouse - male and female - Bone marrow Result: negative (ECHA)

Carcinogenicity

This product is or contains a component that is not classifiable as to its carcinogenicity based on its IARC, ACGIH, NTP, or EPA classification.

- 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 No data available

Specific target organ toxicity - repeated exposure No data available

Aspiration hazard

No data available

Additional Information

Repeated dose toxicity - Pig - male and female - Oral - 42 Days - No observed adverse effect level - >= 61 mg/kg (ECHA)

Repeated dose toxicity - Rat - male and female - Oral - 22 Months - No observed adverse effect level - 25 mg/kg - Lowest observed adverse effect level - 100 mg/kg (ECHA) RTECS: Not available

Depending on the intensity and duration of exposure, effects may vary from mild irritation to severe destruction of tissue., prolonged or repeated exposure can cause:, Damage to the eyes., Nausea, Dizziness, Headache

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

SECTION 12: Ecological information

12.1 Toxicity

Toxicity to fish

semi-static test LC50 - Danio rerio (zebra fish) - > 0.57 mg/l - 96 h (Directive 67/548/EEC, Annex V, C.1.)

Aldrich - 452505

Page 7 of 9



Toxicity to daphnia and other aquatic invertebrates	static test EC50 - Daphnia magna (Water flea) - 0.48 mg/l - 48 h (OECD Test Guideline 202)
Toxicity to algae	static test ErC50 - Desmodesmus subspicatus (green algae) - > 0.4 mg/l - 72 h (Directive 67/548/EEC, Annex V, C.3.)
	static test EC10 - Desmodesmus subspicatus (green algae) - ca. 0.4 mg/l - 72 h (Directive 67/548/EEC, Annex V, C.3.)
Toxicity to bacteria	static test EC50 - activated sludge - > 10,000 mg/l - 3 h (OECD Test Guideline 209)

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

 $\mathsf{PBT}/\mathsf{vPvB}$ assessment not available as chemical safety assessment not required/not conducted

12.6 Other adverse effects

An environmental hazard cannot be excluded in the event of unprofessional handling or disposal.

Very toxic to aquatic life with long lasting effects. No data available

SECTION 13: Disposal considerations

13.1 Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. 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)

Not dangerous goods

IMDG

UN number: 3077 Class: 9 Packing group: III EMS-No: F-A, S-F Proper shipping name: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (2,6-Di(<I>tert</>-butyl-d<SB>9</>)-4-methyl(phenol-3,5,<I>O</>-d<SB>3</>)) Marine pollutant : yes

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Aldrich - 452505

Page 8 of 9



UN number: 3077 Class: 9 Packing group: III Proper shipping name: Environmentally hazardous substance, solid, n.o.s. (2,6-Di(<I>tert</>-butyl-d<SB>9</>)-4-methyl(phenol-3,5,<I>O</>-d<SB>3</>)) **Further information** EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids

SECTION 15: Regulatory information

SARA 302 Components

or > 5kg for solids.

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

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

Acute Health Hazard

Massachusetts Right To Know Components

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

Pennsylvania Right To Know Components

2,6-Di(tert-butyl-d9)-4-methyl(phenol-3,5,0-d3)) CAS-No.	Revision Date
	64502-99-4	1993-02-16

SECTION 16: Other information

Further information

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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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Version: 6.3

Revision Date: 01/21/2020

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Aldrich - 452505

Page 9 of 9

