

SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 6.6

Revision Date 30.08.2024

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

1.1 Product identifiers

Product name : 4-tert-Octylphenol-3,5-d2 solution, 100

Product Number : 32273

Brand : Sigma-Aldrich

Index-No. : 606-001-00-8

REACH No. : This product is a mixture. REACH Registration Number see section 3.

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

Identified uses : Laboratory chemicals, Manufacture of substances

Uses advised against : For R&D use only. Not for pharmaceutical, household or other uses.

1.3

CHEMIKART

1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

SECTION 2: Hazards identification

2.1 Classification of the substance or mixture

Flammable liquids, (Category 2) H225: Highly flammable liquid and vapor.

Eye irritation, (Category 2) H319: Causes serious eye irritation.

Specific target organ toxicity - H336: May cause drowsiness or dizziness.
single exposure, (Category 3),
Central nervous system

2.2 Label elements

Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word Danger

Hazard Statements

H225 Highly flammable liquid and vapor.
H319 Causes serious eye irritation.
H336 May cause drowsiness or dizziness.

Precautionary Statements

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P233 Keep container tightly closed.
P240 Ground and bond container and receiving equipment.
P241 Use explosion-proof electrical/ ventilating/ lighting/ equipment.
P242 Use non-sparking tools.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

Supplemental Hazard information (EU)

EUH066 Repeated exposure may cause skin dryness or cracking.

Reduced Labeling (<= 125 ml)

Pictogram

Signal Word Danger

Hazard Statements none

Precautionary Statements none

Supplemental Hazard information (EU)

EUH066 Repeated exposure may cause skin dryness or cracking.

2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

SECTION 3: Composition/information on ingredients

3.2 Mixtures

Formula : C₁₄D₂H₂₀O
Molecular weight : 208,34 g/mol

Component	Classification	Concentration
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acetone			
CAS-No.	67-64-1	Flam. Liq. 2; Eye Irrit. 2; STOT SE 3; H225, H319, H336	>= 90 - <= 100 %
EC-No.	200-662-2		
Index-No.	606-001-00-8		
Registration number	01-2119471330-49-XXXX	Concentration limits: >= 20 %: STOT SE 3, H336;	
4-tert-Octylphenol-3,5-d2 Included in the Candidate List of Substances of Very High Concern (SVHC) according to Regulation (EC) No. 1907/2006 (REACH)			
CAS-No.	1173021-20-9	Skin Irrit. 2; Eye Dam. 1; Aquatic Acute 1; Aquatic Chronic 1; H315, H318, H400, H410	>= 0,0025 - < 0,025 %
	*	M-Factor - Aquatic Acute: 10 - Aquatic Chronic: 10	

*A registration number is not available for this substance as the substance or its use are exempted from registration according to Article 2 REACH Regulation (EC) No 1907/2006, or the annual tonnage does not require a registration.

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. 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

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.

Pay attention to flashback.

Vapors are heavier than air and may spread along floors.

Development of hazardous combustion gases or vapours possible in the event of fire.

Forms explosive mixtures with air at ambient temperatures.

5.3 Advice for firefighters

In the event of fire, wear self-contained breathing apparatus.

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 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.

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

Change contaminated clothing. Preventive skin protection recommended. Wash hands 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.

Storage stability Recommended storage temperature

-20 °C

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

SECTION 8: Exposure controls/personal protection

8.1 Control parameters

Ingredients with workplace control parameters

8.2 Exposure controls

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). Safety glasses

Skin protection

required

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.

Recommended Filter type: Filter type AX

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.

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) Physical state | liquid |
| b) Color | colorless |
| c) Odor | No data available |
| d) Melting | No data available |

- point/freezing point
- | | |
|---|--|
| e) Initial boiling point and boiling range | 56,0 °C at 1.013 hPa |
| f) Flammability (solid, gas) | No data available |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 13 %(V)
Lower explosion limit: 2 %(V) |
| h) Flash point | -17,0 °C - closed cup |
| i) Autoignition temperature | No data available |
| j) Decomposition temperature | No data available |
| k) pH | No data available |
| l) Viscosity | Viscosity, kinematic: No data available
Viscosity, dynamic: No data available |
| m) Water solubility | No data available |
| n) Partition coefficient: n-octanol/water | No data available |
| o) Vapor pressure | 533,3 hPa at 39,5 °C
245,3 hPa at 20,0 °C |
| p) Density | 0,79 g/cm ³ |
| Relative density | No data available |
| q) Relative vapor density | No data available |
| r) Particle characteristics | No data available |
| s) Explosive properties | Not classified as explosive. |
| t) Oxidizing properties | none |

9.2 Other safety information

No data available

SECTION 10: Stability and reactivity

10.1 Reactivity

Vapors may form explosive mixture with air.

10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

10.3 Possibility of hazardous reactions

Violent reactions possible with:

10.4 Conditions to avoid

Warming.

10.5 Incompatible materials

Bases, Oxidizing agents, Reducing agents, Acetone reacts violently with phosphorous oxychloride.

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

Oral: No data available

Symptoms: Possible symptoms:, mucosal irritations

Dermal: No data available

Skin corrosion/irritation

Remarks: Repeated exposure with the mixture may cause skin dryness or cracking.

Serious eye damage/eye irritation

Remarks: Mixture causes serious eye irritation.

Respiratory or skin sensitization

No data available

Germ cell mutagenicity

No data available

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Mixture may cause drowsiness or dizziness.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

11.2 Additional Information

Endocrine disrupting properties

Product:

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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.

Components

acetone

Acute toxicity

LD50 Oral - Rat - female - 5.800 mg/kg

Remarks: (ECHA)

Symptoms: Stomach/intestinal disorders, Risk of aspiration upon vomiting., Pulmonary failure possible after aspiration of vomit.

LC50 Inhalation - Rat - 4 h - 76 mg/l - vapor

Remarks: Unconsciousness

Drowsiness

Dizziness

(External MSDS)

LD50 Dermal - Rabbit - 20.000 mg/kg

Remarks: (IUCLID)

Skin corrosion/irritation

Skin - Rabbit

Result: Mild skin irritation - 24 h

(Draize Test)

Remarks: (RTECS)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Eye irritation - 24 h

(Draize Test)

Remarks: (RTECS)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: negative

Remarks: (ECHA)

Chronic exposure may cause dermatitis.

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster ovary cells

Result: negative

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: Mouse lymphoma test

Result: negative

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

Inhalation - May cause drowsiness or dizziness. - Narcotic effects

Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Acute oral toxicity - Stomach/intestinal disorders, Risk of aspiration upon vomiting., Pulmonary failure possible after aspiration of vomit.

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

4-tert-Octylphenol-3,5-d2**Acute toxicity**

LD50 Oral - Rat - male and female - 4.040 mg/kg

(OECD Test Guideline 401)

Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Inhalation: No data available

LD50 Dermal - Rabbit - male and female - > 2.000 mg/kg

(OECD Test Guideline 402)

Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 4 h

(OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage. - 24 h

(OECD Test Guideline 405)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Respiratory or skin sensitization

Freund's complete adjuvant test - Guinea pig

Result: negative

(OECD Test Guideline 406)

Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Germ cell mutagenicity

Test Type: Mutagenicity (mammal cell test): chromosome aberration.

Test system: Chinese hamster lung cells

Result: negative

Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Test Type: Ames test

Test system: Salmonella typhimurium

Result: negative

Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Test Type: In vitro mammalian cell gene mutation test

Test system: Chinese hamster ovary cells

Result: negative

Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol

Carcinogenicity

No data available

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

No data available

Specific target organ toxicity - repeated exposure

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

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

12.6 Endocrine disrupting properties

Product:

Assessment : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Components:

4-tert-Octylphenol-3,5-d2:

Assessment : The substance is considered to have endocrine disrupting properties according to REACH Article 57(f) for the environment.

12.7 Other adverse effects

No data available

Components

acetone

Toxicity to fish	flow-through test LC50 - Pimephales promelas (fathead minnow) - 6.210 mg/l - 96 h (OECD Test Guideline 203)
Toxicity to daphnia and other aquatic invertebrates	static test LC50 - Daphnia pulex (Water flea) - 8.800 mg/l - 48 h Remarks: (ECHA)
Toxicity to algae	static test NOEC - M.aeruginosa - 530 mg/l - 8 d (DIN 38412) Remarks: (maximum permissible toxic concentration) (IUCLID)
Toxicity to bacteria	static test EC50 - activated sludge - 61,15 mg/l - 30 min (OECD Test Guideline 209)
Toxicity to daphnia and other aquatic invertebrates(Chronic toxicity)	flow-through test NOEC - Daphnia magna (Water flea) - 2.212 mg/l - 28 d Remarks: (ECHA)

4-tert-Octylphenol-3,5-d2

Toxicity to bacteria	Remarks: The value is given in analogy to the following substances: 4-(1,1,3,3-tetramethylbutyl)phenol
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SECTION 13: Disposal considerations

13.1 Waste treatment methods

No data available

SECTION 14: Transport information

14.1 UN number

ADR/RID: 1090

IMDG: 1090

IATA: 1090

14.2 UN proper shipping name

ADR/RID: ACETONE, SOLUTION

IMDG: ACETONE, SOLUTION

IATA: Acetone, SOLUTION

14.3 Transport hazard class(es)

ADR/RID: 3

IMDG: 3

IATA: 3

14.4 Packaging group

ADR/RID: II

IMDG: II

IATA: II

14.5 Environmental hazards

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

14.6 Special precautions for user

Tunnel restriction code : (D/E)

Further information : No data available

SECTION 15: Regulatory information

15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

Authorisations and/or restrictions on use

Regulation (EU) 2019/1148 on the marketing and use of explosives precursors : acetone

National legislation

Seveso III: Directive 2012/18/EU of the European Parliament and of the Council on the control of major-accident hazards involving dangerous substances. P5c FLAMMABLE LIQUIDS

Other regulations

Take note of Dir 94/33/EC on the protection of young people at work.

15.2 Chemical Safety Assessment

For this product a chemical safety assessment was not carried out

SECTION 16: Other information

Full text of H-Statements

H225	Highly flammable liquid and vapor.
H315	Causes skin irritation.
H318	Causes serious eye damage.
H319	Causes serious eye irritation.
H336	May cause drowsiness or dizziness.
H400	Very toxic to aquatic life.
H410	Very toxic to aquatic life with long lasting effects.
EUH066	Repeated exposure may cause skin dryness or cracking.

Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; 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; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and 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 Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; 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; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization 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; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; 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

Classification of the mixture

Flam. Liq.2	H225
Eye Irrit.2	H319
STOT SE3	H336

Classification procedure:

Based on product data or assessment
Calculation method
Calculation method

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 and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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