

**SAFETY DATA SHEET**

according to Regulation (EC) No. 1907/2006

Version 6.9

Revision Date 30.08.2024

Print Date 02.05.2025

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-ring-<sup>13</sup>C<sub>6</sub> solution

Product Number : 33565

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&amp;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 -  
single exposure, (Category 3),  
Central nervous system H336: May cause drowsiness or dizziness.**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

|          |                                                                 |
|----------|-----------------------------------------------------------------|
| Synonyms | : 4-(1,1,3,3-Tetramethylbutyl)phenol-13C6<br>4-tert-OP-13C6     |
| Formula  | : <sup>13</sup> C <sub>6</sub> C <sub>8</sub> H <sub>22</sub> O |

Molecular weight : 212,28 g/mol

| Component           |                       | Classification                                                                                                         | Concentration    |
|---------------------|-----------------------|------------------------------------------------------------------------------------------------------------------------|------------------|
| <b>acetone</b>      |                       |                                                                                                                        |                  |
| CAS-No.             | 67-64-1               | Flam. Liq. 2; Eye Irrit. 2;<br>STOT SE 3; H225, H319,<br>H336<br>Concentration limits:<br>>= 20 %: STOT SE 3,<br>H336; | >= 90 - <= 100 % |
| EC-No.              | 200-662-2             |                                                                                                                        |                  |
| Index-No.           | 606-001-00-8          |                                                                                                                        |                  |
| Registration number | 01-2119471330-49-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. 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

Combustible.

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. Chemizorb®). 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 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.

##### 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                                         | stinging                                                            |
| d) Melting point/freezing point                 | Melting point: 94,8 °C - Information refers to the main ingredient. |
| e) Initial boiling point and boiling range      | No data available                                                   |
| f) Flammability (solid, gas)                    | No data available                                                   |
| g) Upper/lower flammability or explosive limits | No data available                                                   |
| h) Flash point                                  | -17 °C - Information refers to the main ingredient.                 |
| i) Autoignition temperature                     | No data available                                                   |

- |                                           |                                                                                  |
|-------------------------------------------|----------------------------------------------------------------------------------|
| j) Decomposition temperature              | No data available                                                                |
| k) pH                                     | No data available                                                                |
| l) Viscosity                              | Viscosity, kinematic: No data available<br>Viscosity, dynamic: No data available |
| m) Water solubility                       | No data available                                                                |
| n) Partition coefficient: n-octanol/water | No data available                                                                |
| o) Vapor pressure                         | No data available                                                                |
| p) Density                                | No data available                                                                |
| 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**

Chronic exposure may cause dermatitis.

**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

---

## 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-13C6 (ring-13C6):**

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<br>(OECD Test Guideline 203)                 |
| Toxicity to daphnia and other aquatic invertebrates                   | static test LC50 - Daphnia pulex (Water flea) - 8.800 mg/l - 48 h<br>Remarks: (ECHA)                                           |
| Toxicity to algae                                                     | static test NOEC - M.aeruginosa - 530 mg/l - 8 d<br>(DIN 38412)<br>Remarks: (maximum permissible toxic concentration) (IUCLID) |
| Toxicity to bacteria                                                  | static test EC50 - activated sludge - 61,15 mg/l - 30 min<br>(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<br>Remarks: (ECHA)                                     |

---

## 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.                    |
| H319   | Causes serious eye irritation.                        |
| H336   | May cause drowsiness or dizziness.                    |
| 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](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

Copyright 2020 Sigma-Aldrich Co. LLC. License granted to make unlimited paper copies for internal use only.

The branding on the header and/or footer of this document may temporarily not visually match the product purchased as we transition our branding. However, all of the information in the document regarding the product remains unchanged and matches the product ordered. For further information please contact [mlsbranding@sial.com](mailto:mlsbranding@sial.com).

CHEMIKART