

ALFAAA15612

## 4-tert-Butylcyclohexanone

### SECTION 1. IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING

**产品说明:** 4-叔丁基环己酮  
**Product Description:** 4-tert-Butylcyclohexanone

**Cat No. :** A15612  
**Synonyms** cyclohexanone; 4-(1,1-dimethylethyl); p-tert-butylcyclohexanone  
**CAS No** 98-53-3  
**Molecular Formula** C10 H18 O

**Supplier** Avocado Research Chemicals Ltd.  
(Part of Thermo Fisher Scientific)  
Shore Road, Heysham  
Lancashire, LA3 2XY,  
United Kingdom  
Office Tel: +44 (0) 1524 850506  
Office Fax: +44 (0) 1524 850608

**Emergency Telephone Number** For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11  
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99  
**CHEMTREC** Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

**E-mail address** begel.sdsdesk@thermofisher.com

**Recommended Use** Laboratory chemicals.  
**Uses advised against** No Information available

### SECTION 2. HAZARD IDENTIFICATION

**Physical State**  
Powder Solid

**Appearance**  
Off-white

**Odor**  
Woody

#### Emergency Overview

Harmful if swallowed. Toxic to aquatic life with long lasting effects.

#### Classification of the substance or mixture

|                          |            |
|--------------------------|------------|
| Acute Oral Toxicity      | Category 4 |
| Chronic aquatic toxicity | Category 2 |

#### Label Elements



**Signal Word**

**Warning**

**Hazard Statements**

## 4-tert-Butylcyclohexanone

H302 - Harmful if swallowed

H411 - Toxic to aquatic life with long lasting effects

**Precautionary Statements****Prevention**

P264 - Wash face, hands and any exposed skin thoroughly after handling

P270 - Do not eat, drink or smoke when using this product

**Response**

P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor if you feel unwell

P330 - Rinse mouth

**Storage**

P403 - Store in a well-ventilated place

**Disposal**

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

**Physical and Chemical Hazards**

None identified.

**Health Hazards**

Harmful if swallowed.

**Environmental hazards**

Toxic to aquatic life with long lasting effects. Is not likely mobile in the environment due its low water solubility. Spillage unlikely to penetrate soil.

This product does not contain any known or suspected endocrine disruptors.

**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

| Component                             | CAS No  | Weight % |
|---------------------------------------|---------|----------|
| Cyclohexanone, 4-(1,1-dimethylethyl)- | 98-53-3 | >95      |

**SECTION 4. FIRST AID MEASURES****General Advice**

If symptoms persist, call a physician.

**Eye Contact**

Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.

**Skin Contact**

Get medical attention. Wash off immediately with plenty of water for at least 15 minutes.

**Inhalation**

Remove to fresh air. Get medical attention. If breathing is difficult, give oxygen.

**Ingestion**

Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.

**Most important symptoms and effects**

None reasonably foreseeable.

**Self-Protection of the First Aider**

No special precautions required.

**Notes to Physician**

Treat symptomatically.

**SECTION 5. FIRE-FIGHTING MEASURES**

## 4-tert-Butylcyclohexanone

**Suitable Extinguishing Media**

Water spray, carbon dioxide (CO<sub>2</sub>), dry chemical, alcohol-resistant foam.

**Extinguishing media which must not be used for safety reasons**

No information available.

**Specific Hazards Arising from the Chemical**

Thermal decomposition can lead to release of irritating gases and vapors.

**Protective Equipment and Precautions for Firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear.

**SECTION 6. ACCIDENTAL RELEASE MEASURES****Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required. Avoid dust formation.

**Environmental Precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information. Avoid release to the environment. Collect spillage.

**Methods for Containment and Clean Up**

Sweep up and shovel into suitable containers for disposal. Keep in suitable, closed containers for disposal.

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7. HANDLING AND STORAGE****Handling**

Wear personal protective equipment/face protection. Ensure adequate ventilation. Do not get in eyes, on skin, or on clothing. Avoid ingestion and inhalation. Avoid dust formation.

**Storage**

Keep containers tightly closed in a dry, cool and well-ventilated place.

**Specific Use(s)**

Use in laboratories

**SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION****Control Parameters****Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents. MDHS14/3 General methods for sampling and gravimetric analysis of respirable and inhalable dust MDHS70 General methods for sampling airborne gases and vapours MDHS 96 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Exposure Controls****Engineering Measures**

None under normal use conditions. .

**Personal protective equipment**

## 4-tert-Butylcyclohexanone

|                        |                                                                                 |
|------------------------|---------------------------------------------------------------------------------|
| <b>Eye Protection</b>  | Wear safety glasses with side shields (or goggles) (European standard - EN 166) |
| <b>Hand Protection</b> | Protective gloves                                                               |

| Glove material | Breakthrough time | Glove thickness | EU standard | Glove comments        |
|----------------|-------------------|-----------------|-------------|-----------------------|
| Natural rubber | See manufacturers | -               | EN 374      | (minimum requirement) |
| Nitrile rubber | recommendations   |                 |             |                       |
| Neoprene       |                   |                 |             |                       |
| PVC            |                   |                 |             |                       |

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves.  
(Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion.

Remove gloves with care avoiding skin contamination.

|                                   |                                                                                                                                                                                                        |
|-----------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Skin and body protection</b>   | Long sleeved clothing                                                                                                                                                                                  |
| <b>Respiratory Protection</b>     | No protective equipment is needed under normal use conditions.                                                                                                                                         |
| <b>Large scale/emergency use</b>  | Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced<br><b>Recommended Filter type:</b> Particle filter |
| <b>Small scale/Laboratory use</b> | Maintain adequate ventilation                                                                                                                                                                          |

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice.

**Environmental exposure controls** No information available.

## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

|                                                |                                 |                                          |
|------------------------------------------------|---------------------------------|------------------------------------------|
| <b>Appearance</b>                              | Off-white                       |                                          |
| <b>Physical State</b>                          | Powder Solid                    |                                          |
| <b>Odor</b>                                    | Woody                           |                                          |
| <b>Odor Threshold</b>                          | No data available               |                                          |
| <b>pH</b>                                      | No information available        |                                          |
| <b>Melting Point/Range</b>                     | 48 - 51 °C / 118.4 - 123.8 °F   |                                          |
| <b>Softening Point</b>                         | No data available               |                                          |
| <b>Boiling Point/Range</b>                     | 113 - 116 °C / 235.4 - 240.8 °F | @ 20 mmHg                                |
| <b>Flash Point</b>                             | 96 °C / 204.8 °F                | <b>Method -</b> No information available |
| <b>Evaporation Rate</b>                        | Not applicable                  | Solid                                    |
| <b>Flammability (solid,gas)</b>                | No information available        |                                          |
| <b>Explosion Limits</b>                        | No data available               |                                          |
| <b>Vapor Pressure</b>                          | No data available               |                                          |
| <b>Vapor Density</b>                           | Not applicable                  | Solid                                    |
| <b>Specific Gravity / Density</b>              | No data available               |                                          |
| <b>Bulk Density</b>                            | No data available               |                                          |
| <b>Water Solubility</b>                        | Insoluble                       |                                          |
| <b>Solubility in other solvents</b>            | No information available        |                                          |
| <b>Partition Coefficient (n-octanol/water)</b> |                                 |                                          |
| <b>Autoignition Temperature</b>                | No data available               |                                          |
| <b>Decomposition Temperature</b>               | No data available               |                                          |
| <b>Viscosity</b>                               | Not applicable                  | Solid                                    |
| <b>Explosive Properties</b>                    | No information available        |                                          |
| <b>Oxidizing Properties</b>                    | No information available        |                                          |

## 4-tert-Butylcyclohexanone

Molecular Formula C10 H18 O  
Molecular Weight 154.25

## SECTION 10. STABILITY AND REACTIVITY

**Stability** Stable under normal conditions.

**Hazardous Reactions** None under normal processing.

**Hazardous Polymerization** Hazardous polymerization does not occur.

**Conditions to Avoid** Incompatible products. Excess heat. Avoid dust formation.

**Materials to avoid** Strong oxidizing agents.

**Hazardous Decomposition Products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11. TOXICOLOGICAL INFORMATION

## Product Information

## (a) acute toxicity;

| Component                             | LD50 Oral              | LD50 Dermal | LC50 Inhalation |
|---------------------------------------|------------------------|-------------|-----------------|
| Cyclohexanone, 4-(1,1-dimethylethyl)- | 300-2000 mg/kg ( Rat ) |             |                 |

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

## (d) respiratory or skin sensitization;

Respiratory No data available  
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity; No data available

There are no known carcinogenic chemicals in this product

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; Not applicable  
Solid

**Other Adverse Effects** The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information

## 4-tert-Butylcyclohexanone

Symptoms / effects, both acute and delayed No information available

## SECTION 12. ECOLOGICAL INFORMATION

## Ecotoxicity effects

Do not empty into drains.

Persistence and Degradability  
Persistence

Insoluble in water, Persistence is unlikely, based on information available.

## Bioaccumulative Potential

May have some potential to bioaccumulate

## Mobility in soil

Spillage unlikely to penetrate soil Is not likely mobile in the environment due its low water solubility

Endocrine Disruptor Information  
Persistent Organic Pollutant  
Ozone Depletion Potential

This product does not contain any known or suspected endocrine disruptors  
This product does not contain any known or suspected substance  
This product does not contain any known or suspected substance

## SECTION 13. DISPOSAL CONSIDERATIONS

## Waste from Residues/Unused Products

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

## Contaminated Packaging

Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.

## Other Information

Waste codes should be assigned by the user based on the application for which the product was used.

## SECTION 14. TRANSPORT INFORMATION

## Road and Rail Transport

Not Regulated

## IMDG/IMO

Not regulated

## IATA

Not regulated

## Special Precautions for User

No special precautions required

## SECTION 15. REGULATORY INFORMATION

## International Inventories

X = listed, China (IECSC), Europe (EINECS/ELINCS/NLP), U.S.A. (TSCA), Canada (DSL/NDSL), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), Korea (KECL).

| Component | The Inventory of Hazardous Goods | List of dangerous goods GB | TCSI | IECSC | EINECS | TSCA | DSL | PICCS | ENCS | ISHL | AICS | KECL |
|-----------|----------------------------------|----------------------------|------|-------|--------|------|-----|-------|------|------|------|------|
|           |                                  |                            |      |       |        |      |     |       |      |      |      |      |

**SAFETY DATA SHEET****4-tert-Butylcyclohexanone**

|                                          | Chemicals<br>(2015<br>Edition) | 12268 -<br>2012 |   |   |           |   |   |   |   |   |   |          |
|------------------------------------------|--------------------------------|-----------------|---|---|-----------|---|---|---|---|---|---|----------|
| Cyclohexanone,<br>4-(1,1-dimethylethyl)- | -                              | -               | X | X | 202-678-5 | X | X | X | X | X | X | KE-04258 |

**National Regulations****SECTION 16. OTHER INFORMATION**

**Prepared By** Health, Safety and Environmental Department  
**Creation Date** 27-Mar-2014  
**Revision Date** 07-Sep-2025  
**Revision Summary** Not applicable.

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.

**Legend**

**CAS** - Chemical Abstracts Service

**EINECS/ELINCS** - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances

**PICCS** - Philippines Inventory of Chemicals and Chemical Substances

**IECSC** - Chinese Inventory of Existing Chemical Substances

**KECL** - Korean Existing and Evaluated Chemical Substances

**TSCA** - United States Toxic Substances Control Act Section 8(b) Inventory

**DSL/NDSL** - Canadian Domestic Substances List/Non-Domestic Substances List

**ENCS** - Japanese Existing and New Chemical Substances

**AICS** - Australian Inventory of Chemical Substances

**NZIoC** - New Zealand Inventory of Chemicals

**WEL** - Workplace Exposure Limit

**ACGIH** - American Conference of Governmental Industrial Hygienists

**DNEL** - Derived No Effect Level

**RPE** - Respiratory Protective Equipment

**LC50** - Lethal Concentration 50%

**NOEC** - No Observed Effect Concentration

**PBT** - Persistent, Bioaccumulative, Toxic

**TWA** - Time Weighted Average

**IARC** - International Agency for Research on Cancer

**PNEC** - Predicted No Effect Concentration

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

**ICAO/IATA** - International Civil Aviation Organization/International Air Transport Association

**ADR** - European Agreement Concerning the International Carriage of Dangerous Goods by Road

**OECD** - Organisation for Economic Co-operation and Development

**BCF** - Bioconcentration factor

**IMO/IMDG** - International Maritime Organization/International Maritime Dangerous Goods Code

**MARPOL** - International Convention for the Prevention of Pollution from Ships

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

**Key literature references and sources for data**

<https://echa.europa.eu/information-on-chemicals>

Suppliers safety data sheet, Chemadvisor - LOLI, Merck index, RTECS

**Disclaimer**

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

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**End of Safety Data Sheet**