

Creation Date 27-Mar-2014

Revision Date 26-Jan-2024

Revision Number 3

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

### 1.1. Product identifier

Product Description:	<b>4-tert-Butylcyclohexanone</b>
Cat No. :	<b>A15612</b>
Synonyms	cyclohexanone; 4-(1,1-dimethylethyl); p-tert-butylcyclohexanone
CAS No	98-53-3
EC No	202-678-5
Molecular Formula	C <sub>10</sub> H <sub>18</sub> O
REACH registration number	-

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

Recommended Use	Laboratory chemicals.
Uses advised against	No Information available

### 1.3. Details of the supplier of the safety data sheet

Company	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
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E-mail address	begel.sdsdesk@thermofisher.com
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### 1.4. 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

## SECTION 2: HAZARDS IDENTIFICATION

### 2.1. Classification of the substance or mixture

#### CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567

#### Physical hazards

Based on available data, the classification criteria are not met

#### Health hazards

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

Acute oral toxicity

Category 4 (H302)

## **Environmental hazards**

Chronic aquatic toxicity

Category 2 (H411)

Full text of Hazard Statements: see section 16

## **2.2. Label elements**



Signal Word

Warning

## **Hazard Statements**

H302 - Harmful if swallowed

H411 - Toxic to aquatic life with long lasting effects

## **Precautionary Statements**

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

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

P273 - Avoid release to the environment

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

P391 - Collect spillage

## **2.3. Other hazards**

This product does not contain any known or suspected endocrine disruptors

## **SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS**

### **3.1. Substances**

Component	CAS No	EC No	Weight %	CLP Classification - According to GB-CLP Regulations UK SI 2019/720 and UK SI 2020/1567
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	EEC No. 202-678-5	>95	Acute Tox. 4 (H302) Aquatic Chronic 2 (H411)

REACH registration number

-

Full text of Hazard Statements: see section 16

## **SECTION 4: FIRST AID MEASURES**

### **4.1. Description of first aid measures**

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

<b>General Advice</b>	If symptoms persist, call a physician.
<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention.
<b>Skin Contact</b>	Get medical attention. Wash off immediately with plenty of water for at least 15 minutes.
<b>Ingestion</b>	Clean mouth with water and drink afterwards plenty of water. Get medical attention if symptoms occur.
<b>Inhalation</b>	Remove to fresh air. Get medical attention. If breathing is difficult, give oxygen.
<b>Self-Protection of the First Aider</b>	No special precautions required.

## **4.2. Most important symptoms and effects, both acute and delayed**

None reasonably foreseeable.

## **4.3. Indication of any immediate medical attention and special treatment needed**

**Notes to Physician** Treat symptomatically.

## **SECTION 5: FIREFIGHTING MEASURES**

### **5.1. Extinguishing media**

#### **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.

### **5.2. Special hazards arising from the substance or mixture**

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

#### **Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

### **5.3. Advice 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**

### **6.1. Personal precautions, protective equipment and emergency procedures**

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

### **6.2. Environmental precautions**

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

### **6.3. Methods and material for containment and cleaning up**

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

### **6.4. Reference to other sections**

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

Refer to protective measures listed in Sections 8 and 13.

## SECTION 7: HANDLING AND STORAGE

### 7.1. Precautions for safe 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.

#### **Hygiene Measures**

Handle in accordance with good industrial hygiene and safety practice.

### 7.2. Conditions for safe storage, including any incompatibilities

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

**Technical Rules for Hazardous Substances (TRGS) 510**      Class 11  
**Storage Class (LGK) (Germany)**

### 7.3. Specific end use(s)

Use in laboratories

## SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION

### 8.1. Control parameters

#### **Exposure limits**

This product, as supplied, does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies

#### **Biological limit values**

This product, as supplied, does not contain any hazardous materials with biological limits established by the region specific regulatory bodies

#### **Derived No Effect Level (DNEL) / Derived Minimum Effect Level (DMEL)**

No information available

#### **Predicted No Effect Concentration (PNEC)**

No information available.

### 8.2. Exposure controls

#### **Engineering Measures**

None under normal use conditions.

#### **Personal protective equipment**

##### **Eye Protection**

Wear safety glasses with side shields (or goggles) (European standard - EN 166)

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

<b>Hand Protection</b>		Protective gloves		
<b>Glove material</b>	<b>Breakthrough time</b>	<b>Glove thickness</b>	<b>EU standard</b>	<b>Glove comments</b>
Natural rubber	See manufacturers	-	EN 374	(minimum requirement)
Nitrile rubber	recommendations			
Neoprene				
PVC				

**Skin and body protection** Long sleeved clothing.

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 compatability, 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.

**Respiratory Protection** No protective equipment is needed under normal use conditions.

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced  
**Recommended Filter type:** Particle filter

**Small scale/Laboratory use** Maintain adequate ventilation

**Environmental exposure controls** No information available.

## SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES

### 9.1. Information on basic physical and chemical properties

<b>Physical State</b>	Powder Solid	
<b>Appearance</b>	Off-white	
<b>Odor</b>	Woody	
<b>Odor Threshold</b>	No data 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>Flammability (liquid)</b>	Not applicable	Solid
<b>Flammability (solid,gas)</b>	No information available	
<b>Explosion Limits</b>	No data available	
<b>Flash Point</b>	96 °C / 204.8 °F	<b>Method -</b> No information available
<b>Autoignition Temperature</b>	No data available	
<b>Decomposition Temperature</b>	No data available	
<b>pH</b>	No information available	
<b>Viscosity</b>	Not applicable	Solid
<b>Water Solubility</b>	Insoluble	
<b>Solubility in other solvents</b>	No information available	
<b>Partition Coefficient (n-octanol/water)</b>		
<b>Vapor Pressure</b>	No data available	
<b>Density / Specific Gravity</b>	No data available	
<b>Bulk Density</b>	No data available	
<b>Vapor Density</b>	Not applicable	Solid
<b>Particle characteristics</b>	No data available	

### 9.2. Other information

**Molecular Formula** C10 H18 O  
**Molecular Weight** 154.25

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

Evaporation Rate Not applicable - Solid

## SECTION 10: STABILITY AND REACTIVITY

**10.1. Reactivity** None known, based on information available

**10.2. Chemical stability** Stable under normal conditions.

### **10.3. Possibility of hazardous reactions**

**Hazardous Polymerization** Hazardous polymerization does not occur.  
**Hazardous Reactions** None under normal processing.

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

**10.5. Incompatible materials** Strong oxidizing agents.

**10.6. Hazardous decomposition products** Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>).

## SECTION 11: TOXICOLOGICAL INFORMATION

### **11.1. Information on hazard classes as defined in Regulation (EC) No 1272/2008**

#### **Product Information**

**(a) acute toxicity;**  
**Oral** Category 4  
**Dermal** Based on available data, the classification criteria are not met  
**Inhalation** Based on available data, the classification criteria are not met

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

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

(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
Symptoms / effects, both acute and delayed	No information available.

## 11.2. Information on other hazards

Endocrine Disrupting Properties	Assess endocrine disrupting properties for human health. This product does not contain any known or suspected endocrine disruptors.
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## SECTION 12: ECOLOGICAL INFORMATION

### 12.1. Toxicity

Ecotoxicity effects	Do not empty into drains.
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### 12.2. Persistence and degradability

Persistence	Insoluble in water, Persistence is unlikely, based on information available.
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### 12.3. Bioaccumulative potential

May have some potential to bioaccumulate

### 12.4. Mobility in soil

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

### 12.5. Results of PBT and vPvB assessment

No data available for assessment.

### 12.6. Endocrine disrupting properties

Endocrine Disruptor Information	This product does not contain any known or suspected endocrine disruptors
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### 12.7. Other adverse effects Persistent Organic Pollutant Ozone Depletion Potential

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

## SECTION 13: DISPOSAL CONSIDERATIONS

### 13.1. Waste treatment methods

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.
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# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

<b>Contaminated Packaging</b>	Empty remaining contents. Dispose of in accordance with local regulations. Do not re-use empty containers.
<b>European Waste Catalogue (EWC)</b>	According to the European Waste Catalog, Waste Codes are not product specific, but application specific.
<b>Other Information</b>	Waste codes should be assigned by the user based on the application for which the product was used.

## SECTION 14: TRANSPORT INFORMATION

**IMDG/IMO** Not regulated

14.1. UN number  
14.2. UN proper shipping name  
14.3. Transport hazard class(es)  
14.4. Packing group

**ADR** Not regulated

14.1. UN number  
14.2. UN proper shipping name  
14.3. Transport hazard class(es)  
14.4. Packing group

**IATA** Not regulated

14.1. UN number  
14.2. UN proper shipping name  
14.3. Transport hazard class(es)  
14.4. Packing group

14.5. Environmental hazards No hazards identified

14.6. Special precautions for user No special precautions required.

14.7. Maritime transport in bulk according to IMO instruments Not applicable, packaged goods

## SECTION 15: REGULATORY INFORMATION

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

#### **International Inventories**

Europe (EINECS/ELINCS/NLP), China (IECSC), Taiwan (TCSI), Korea (KECL), Japan (ENCS), Japan (ISHL), Canada (DSL/NDSL), Australia (AICS), New Zealand (NZIoC), Philippines (PICCS). US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

Component	CAS No	EINECS	ELINCS	NLP	IECSC	TCSI	KECL	ENCS	ISHL
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	202-678-5	-	-	X	X	KE-04258	X	X

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	DSL	NDSL	AICS	NZIoC	PICCS
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	X	ACTIVE	X	-	X	X	X



# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

Legend: X - Listed '-' - Not Listed

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

Authorisation/Restrictions according to EU REACH

Not applicable

Component	CAS No	REACH (1907/2006) - Annex XIV - Substances Subject to Authorization	REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances	REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC)
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	-	-	-

Seveso III Directive (2012/18/EC)

Component	CAS No	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification	Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	Not applicable	Not applicable

Regulation (EC) No 649/2012 of the European Parliament and of the Council of 4 July 2012 concerning the export and import of dangerous chemicals

Not applicable

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work .

National Regulations

UK - Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

WGK Classification

See table for values

Component	Germany - Water Classification (AwSV)	Germany - TA-Luft Class
Cyclohexanone, 4-(1,1-dimethylethyl)-	WGK2	

## 15.2. Chemical safety assessment

A Chemical Safety Assessment/Report (CSA/CSR) has not been conducted

## SECTION 16: OTHER INFORMATION

Full text of H-Statements referred to under sections 2 and 3

H302 - Harmful if swallowed

H411 - Toxic to aquatic life with long lasting effects

Legend

# SAFETY DATA SHEET

4-tert-Butylcyclohexanone

Revision Date 26-Jan-2024

**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/NDL** - 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 Predicted No Effect Concentration (PNEC)

**LD50** - Lethal Dose 50%

**EC50** - Effective Concentration 50%

**POW** - Partition coefficient Octanol:Water

**vPvB** - very Persistent, very Bioaccumulative

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

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

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

**BCF** - Bioconcentration factor

**Key literature references and sources for data**

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

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

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

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

**ATE** - Acute Toxicity Estimate

**VOC** - (Volatile Organic Compound)

## Training Advice

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

**Prepared By**

Health, Safety and Environmental Department

**Creation Date**

27-Mar-2014

**Revision Date**

26-Jan-2024

**Revision Summary**

New emergency telephone response service provider.

**This safety data sheet complies with Regulation UK SI 2019/758 and UK SI 2020/1577 as amended.**

## 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

**End of Safety Data Sheet**