# Thermo Fisher SCIENTIFIC

# SAFETY DATA SHEET

Page 1/7
Revision Date 26-Apr-2024
Version 3

ALFAAA12832

# 4-tert-Pentylcyclohexanone

### 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-Pentylcyclohexanone

Cat No. : A12832

Synonyms 4-tert-Amylcyclohexanone; Cyclohexanone, 4-(1,1-Dimethylpropyl)-; 4-(1,1-Dimethylpropyl)

CAS No 16587-71-6 Molecular Formula C11H20O

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 StateAppearanceOdorLiquidColorlesssweet

**Emergency Overview** 

May be harmful if swallowed. May be harmful in contact with skin.

### Classification of the substance or mixture

Acute Oral Toxicity	Category 5
Acute Dermal Toxicity	Category 5

#### **Label Elements**

None required

#### **Hazard Statements**

H303 - May be harmful if swallowed H313 - May be harmful in contact with skin

### **Precautionary Statements**

Prevention

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

Page 2/7 Revision Date 26-Apr-2024

### 4-tert-Pentylcyclohexanone

P280 - Wear protective gloves

Response

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

#### **Physical and Chemical Hazards**

None identified.

**Health Hazards** 

May be harmful if swallowed. May be harmful in contact with skin.

#### **Environmental hazards**

Contains no substances known to be hazardous to the environment or not degradable in waste water treatment plants.

Toxic to terrestrial vertebrates. 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-dimethylpropyl)-	16587-71-6	> 98		

#### **SECTION 4. FIRST AID MEASURES**

#### **Eye Contact**

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

#### Skin Contact

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

#### Inhalation

Remove to fresh air. Get medical attention immediately if symptoms occur.

#### 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**

#### Suitable Extinguishing Media

Use extinguishing measures that are appropriate to local circumstances and the surrounding environment.

#### 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**

Page 3/7 Revision Date 26-Apr-2024

### 4-tert-Pentylcyclohexanone

#### **Personal Precautions**

Ensure adequate ventilation. Use personal protective equipment as required.

#### **Environmental Precautions**

Should not be released into the environment. See Section 12 for additional Ecological Information.

#### Methods for Containment and Clean Up

Sweep up and shovel into suitable 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. Avoid contact with skin, eyes or clothing. Avoid ingestion and inhalation.

#### Storage

Keep container tightly closed in a dry and well-ventilated place.

#### Specific Use(s)

Use in laboratories

### **SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION**

#### **Control Parameters**

#### **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)

Hand Protection Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Disposable gloves	See manufacturers	-	EN 374	(minimum requirement)
	recommendations			

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.

Skin and body protection Long sleeved clothing

**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

Page 4/7 Revision Date 26-Apr-2024

### 4-tert-Pentylcyclohexanone

Small scale/Laboratory use 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**

Appearance Colorless Physical State Liquid

**Odor** sweet

Odor Threshold No data available

рΗ

Melting Point/RangeNo data availableSoftening PointNo data available

**Boiling Point/Range** 124 - 125 °C / 255.2 - 257 °F @ 16 mmHg

Flash Point 104 °C / 219.2 °F Method - No information available

**Evaporation Rate** No data available

Flammability (solid,gas) Not applicable Liquid

Explosion Limits No data available

Vapor Pressure No data available

Vapor Density 5.80 (Air = 1.0)

Specific Gravity / Density .9200

Bulk Density Not applicable Liquid

Water Solubility

No information available
Solubility in other solvents

No information available

Partition Coefficient (n-octanol/water)

Componentlog PowCyclohexanone,3.9

4-(1,1-dimethylpropyl)-

Autoignition Temperature
Decomposition Temperature
Viscosity

No data available
No data available
No data available

**Explosive Properties**Oxidizing Properties
No information available
No information available

Molecular Formula C11H20O Molecular Weight 168.28

### **SECTION 10. STABILITY AND REACTIVITY**

**Stability** Stable under normal conditions.

Hazardous ReactionsNone under normal processing.Hazardous PolymerizationNo information available.

Conditions to Avoid None known.

Materials to avoid No information available.

Hazardous Decomposition Products None under normal use conditions.

## **SECTION 11. TOXICOLOGICAL INFORMATION**

Page 5/7 Revision Date 26-Apr-2024

### 4-tert-Pentylcyclohexanone

\_\_\_\_\_

#### **Product Information**

(a) acute toxicity;

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation			
Cyclohexanone, 4-(1,1-dimethylpropyl)-	LD50 = 4700 mg/kg (Rat)	LD50 = 4700 mg/kg (Rabbit)				

(b) skin corrosion/irritation; No data available

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

(d) respiratory or skin sensitization;

**Respiratory**Skin
No data available
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 None known.

(j) aspiration hazard; No data available

Symptoms / effects,both acute and No information available

delayed

# **SECTION 12. ECOLOGICAL INFORMATION**

Ecotoxicity effects

Persistence and Degradability

Persistence

No information available Persistence is unlikely.

Bioaccumulative Potential Bioaccumulation is unlikely

Component	log Pow	Bioconcentration factor (BCF)				
Cyclohexanone, 4-(1,1-dimethylpropyl)-	3.9	No data available				

Mobility in soil No information available

**Endocrine Disruptor Information Persistent Organic Pollutant** 

This product does not contain any known or suspected endocrine disruptors

This product does not contain any known or suspected substance

Page 6 / 7 Revision Date 26-Apr-2024

### 4-tert-Pentylcyclohexanone

Ozone Depletion Potential 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 Chemicals (2015 Edition)		TCSI	IECSC	EINECS	TSCA	DSL	PICCS	ENCS	ISHL	AICS	KECL
Cyclohexanone,	-	-	Х	Х	240-642-0	Х	Х	Х	Х	Х	Х	-
4-(1,1-dimethylpropyl)-												

#### **National Regulations**

### **SECTION 16. OTHER INFORMATION**

Prepared By Health, Safety and Environmental Department

Revision Date 26-Apr-2024

**Revision Summary** New emergency telephone response service provider.

### **Training Advice**

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

Page 7/7 Revision Date 26-Apr-2024

### 4-tert-Pentylcyclohexanone

#### Legend

Substances List

**CAS** - Chemical Abstracts Service

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

EINECS/ELINCS - European Inventory of Existing Commercial Chemical DSL/NDSL - Canadian Domestic Substances List/Non-Domestic 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 **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

**End of Safety Data Sheet**