

SAFETY DATA SHEET

Creation Date 27-Mar-2014

Revision Date 27-Mar-2024

Revision Number 3

1. Identification

Product Name 4-tert-Butylcyclohexanone

Cat No. : A15612

CAS No 98-53-3
Synonyms cyclohexanone; 4-(1,1-dimethylethyl); p-tert-butylcyclohexanone

Recommended Use Laboratory chemicals.
Uses advised against Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Thermo Fisher Scientific Chemicals, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Tel: 800-343-0660
Fax: 800-322-4757

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

2. Hazard(s) identification

Classification

This chemical is considered hazardous by the 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute oral toxicity

Category 4

Label Elements

Signal Word

Warning

Hazard Statements

Harmful if swallowed

**Precautionary Statements****Prevention**

Wash face, hands and any exposed skin thoroughly after handling
Do not eat, drink or smoke when using this product

Ingestion

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell
Rinse mouth

Disposal

Dispose of contents/container to an approved waste disposal plant

Hazards not otherwise classified (HNOC)

Toxic to aquatic life with long lasting effects

3. Composition/Information on Ingredients

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

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.
Notes to Physician	Treat symptomatically

5. Fire-fighting measures

Suitable Extinguishing Media	Water spray, carbon dioxide (CO2), dry chemical, alcohol-resistant foam.
Unsuitable Extinguishing Media	No information available
Flash Point	96 °C / 204.8 °F
Method -	No information available
Autoignition Temperature	No information available
Explosion Limits	
Upper	No data available

Lower	No data available
Sensitivity to Mechanical Impact	No information available
Sensitivity to Static Discharge	No information available

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

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.

NFPA

Health
2

Flammability
1

Instability
0

Physical hazards
N/A

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.

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. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures None under normal use conditions.

Personal Protective Equipment

Eye/face Protection Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

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

Recommended Filter type: Particle filter.

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

9. Physical and chemical properties

Physical State Powder Solid

Appearance	Off-white
Odor	Woody
Odor Threshold	No information available
pH	No information available
Melting Point/Range	48 - 51 °C / 118.4 - 123.8 °F
Boiling Point/Range	113 - 116 °C / 235.4 - 240.8 °F @ 20 mmHg
Flash Point	96 °C / 204.8 °F
Evaporation Rate	Not applicable
Flammability (solid,gas)	No information available
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	Not applicable
Specific Gravity	No information available
Solubility	Insoluble in water
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	No information available
Decomposition Temperature	No information available
Viscosity	Not applicable
Molecular Formula	C10 H18 O
Molecular Weight	154.25

10. Stability and reactivity

Reactive Hazard	None known, based on information available
Stability	Stable under normal conditions.
Conditions to Avoid	Incompatible products. Excess heat. Avoid dust formation.
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition Products	Carbon monoxide (CO), Carbon dioxide (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
Cyclohexanone, 4-(1,1-dimethylethyl)-	300-2000 mg/kg (Rat)	Not listed	Not listed

Toxicologically Synergistic Products No information available

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation	No information available
Sensitization	No information available
Carcinogenicity	The table below indicates whether each agency has listed any ingredient as a carcinogen.

Component	CAS No	IARC	NTP	ACGIH	OSHA	Mexico
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	Not listed	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects	No information available
Reproductive Effects	No information available.
Developmental Effects	No information available.
Teratogenicity	No information available.
STOT - single exposure	None known
STOT - repeated exposure	None known
Aspiration hazard	No information available
Symptoms / effects, both acute and delayed	No information available
Endocrine Disruptor Information	No information available
Other Adverse Effects	The toxicological properties have not been fully investigated. See actual entry in RTECS for complete information.

12. Ecological information

Ecotoxicity

Do not empty into drains.

Persistence and Degradability	Insoluble in water Persistence is unlikely based on information available.
Bioaccumulation/ Accumulation	No information available.
Mobility	Is not likely mobile in the environment due its low water solubility.

13. Disposal considerations

Waste Disposal Methods	Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.
-------------------------------	---

14. Transport information

DOT	Not regulated
TDG	Not regulated
IATA	Not regulated
IMDG/IMO	Not regulated

15. Regulatory information

United States of America Inventory

Component	CAS No	TSCA	TSCA Inventory notification - Active-Inactive	TSCA - EPA Regulatory Flags
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	X	ACTIVE	-

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

Component	CAS No	DSL	NDSL	EINECS	PICCS	ENCS	ISHL	AICS	IECSC	KECL
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	X	-	202-678-5	X	X	X	X	X	KE-04258

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

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade Slight risk, Grade 1

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	REACH Regulation (EC 1907/2006) article 59 - Candidate List of
-----------	--------	---	--	--

			Substances	Substances of Very High Concern (SVHC)
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	-	-	-

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

Component	CAS No	OECD HPV	Persistent Organic Pollutant	Ozone Depletion Potential	Restriction of Hazardous Substances (RoHS)
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	Not applicable	Not applicable	Not applicable	Not applicable

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

Not applicable

Other International Regulations

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	Rotterdam Convention (PIC)	Basel Convention (Hazardous Waste)
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	Not applicable	Not applicable	Not applicable	Not applicable

16. Other information

Prepared By

Health, Safety and Environmental Department
 Email: chem.techinfo@thermofisher.com
 www.thermofisher.com

Creation Date

27-Mar-2014

Revision Date

27-Mar-2024

Print Date

27-Mar-2024

Revision Summary

New emergency telephone response service provider.

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 SDS