Chemical Safety Data Sheet MSDS / SDS

4-(1,1,3,3-tetramethylbutyl)phenol SDS

Revision Date:2024-04-25 Revision Number:1

SECTION 1: Identification of the substance/mixture and of the company/undertaking

Product identifier

Product name: 4-(1,1,3,3-tetramethylbutyl)phenol

CAS: 140-66-9

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

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SECTION 2: Hazards identification

Classification of the substance or mixture

Skin irritation, Category 2
Serious eye damage, Category 1

Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H315 Causes skin irritation
H318 Causes serious eye damage
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P273 Avoid release to the environment.

Response

P302+P352 IF ON SKIN: Wash with plenty of water/...
P321 Specific treatment (see ... on this label).
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P317 Get medical help.
P391 Collect spillage.

Storage

none

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	4-(1,1,3,3-tetramethylbutyl)phenol
Common names and synonyms:	4-(1,1,3,3-tetramethylbutyl)phenol
CAS number:	140-66-9
EC number:	205-426-2
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

no data available

Indication of immediate medical attention and special treatment needed, if necessary

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Use dry chemical, carbon dioxide or alcohol-resistant foam.

Specific hazards arising from the chemical

no data available

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours.Avoid contacting with skin and eye. Use personal protective equipment.Wear chemical impermeable gloves. Ensure adequate ventilation.Remove all sources of ignition. Evacuate personnel to safe areas.Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	4-(1,1,3,3-tetramethylbutyl)phenol			
CAS No.	140-66-9			
	Limit value - Eight hours		**Limit value - Short term**	
	ppm	**mg/m^3**	**ppm**	**mg/m^3**
Germany (DFG)	0,5 (1)	4,3 (1)	0,5 (1)(2)	4,3 (1)(2)
Switzerland	0,5	4,3	0,5 (1)	4,3 (1)
	Remarks			
Germany (DFG)	(1) Inhalable fraction and vapour (2) 15 minutes average value			
Switzerland	(1) 15 minutes average value			

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Flakes.
Colour:	White.
Odour:	no data available
Melting point/freezing point:	85 °C. Atm. press.:Ca. 1 atm.
Boiling point or initial boiling point and boiling range:	289 °C. Atm. press.:Ca. 101 kPa.
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	85°C(lit.)
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available

pH:	no data available
Kinematic viscosity:	no data available
Solubility:	In water: 7 mg/L. Temperature: 20 °C. pH: > 6 - < 7.
Partition coefficient n-octanol/water:	log Pow = 4.8. Temperature: 22 °C.
Vapour pressure:	0.02 mBar. Temperature: 38 °C.
Density and/or relative density:	0.37 g/cm3. Temperature: 22 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

no data available

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomp it emits acrid smoke and fumes.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - 4 040 mg/kg bw.

Inhalation: LC100 - rat - 116 mg/L air.

Dermal: LD50 - rabbit - > 2 000 mg/kg bw.

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Leuciscus idus melanotus - 0.26 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC50 - Gammarus pulex - 19.6 µg/L - 96 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 1.9 mg/L - 96 h.

Toxicity to microorganisms: EC50 - a mixed population of activated sewage sludge microorganisms - > 10 mg/L - 3 h.
Remarks:Respiration rate.

Persistence and degradability

In experiments with a soil column, concentrations of 4-(1,1,3,3-tetramethylbutyl)phenol were about two orders of magnitude lower in the column effluent than in the feed(1). Soil from this column, which had undergone 3 inundation cycles with 4-(1,1,3,3-tetramethylbutyl)phenol at 10 ug/l, required 16 hours to convert 7% of this compound to CO2. Microbial adaptation was noted for this compound, as indicated by increased removal efficiencies during successive inundation cycles (6 day flooding, 16 day drying cycle) at varying concentrations. Column effluent concentrations of 4-(1,1,3,3-tetramethylbutyl)phenol were independent of input concentrations during the final stage of the test(1). Following three aerobic flooding cycles, anaerobic conditions were introduced(2). Fractional breakthrough profiles for 4-(1,1,3,3-tetramethylbutyl)phenol did not change (from those obtained during aerobic test conditions) although the degree of breakthrough increased for this compound; this indicates that the inhibition in compound removal mediated by anaerobic conditions is not due solely to cessation of mineralization activity(2).

Bioaccumulative potential

An estimated BCF value of 6000 was calculated for 4-(1,1,3,3-tetramethylbutyl)phenol(SRC), using an estimated log Kow of 5.28(1,SRC) and a recommended regression-derived equation(2). According to a recommended classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms will be an important fate process(SRC).

Mobility in soil

The Koc of 4-(1,1,3,3-tetramethylbutyl)phenol is estimated as approximately 18,000(SRC), using an estimated log Kow of 5.28(1,SRC) and a regression-derived equation(2,SRC). According to a recommended classification scheme(3), this estimated Koc value suggests that 4-(1,1,3,3-tetramethylbutyl)phenol will be immobile in soil(SRC). However, this compound was measured in wells down gradient from the flooding basins (0.17 ug/L) during rapid infiltration of primary sewage (containing 4-(1,1,3,3-tetramethylbutyl)phenol at 0.79 ug/L) at a kame site(4). Sorption processes did not appear to completely control the movement of this compound through soil(4). This compound was again present in wells down gradient from the initial site(at 0.01-0.017 ug/L) at another rapid infiltration site in Arizona (4-(1,1,3,3-tetramethylbutyl)phenol initially present at 0.757 ug/L); here, removal of 4-(1,1,3,3-tetramethylbutyl)phenol was attributed mainly to sorption processes as the sewage had been through secondary treatment(5).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Environmental hazards

ADR/RID: Yes
IMDG: Yes
IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

IPCS - The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home

HSDB - Hazardous Substances Data Bank, website: https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm

IARC - International Agency for Research on Cancer, website: http://www.iarc.fr/

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple

ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: http://www.phmsa.dot.gov/hazmat/library/erg

Germany GESTIS-database on hazard substance, website: http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp

ECHA - European Chemicals Agency, website: https://echa.europa.eu/