Chemical Safety Data Sheet MSDS / SDS

2,6-di-tert-butylphenol 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: 2,6-di-tert-butylphenol

CAS: 128-39-2

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

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

Telephone: +91 9550333722

SECTION 2: Hazards identification

Classification of the substance or mixture

Skin irritation, Category 2
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 Warning

Hazard statement(s)

H315 Causes skin irritation
H400 Very toxic to aquatic life
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.
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:	2,6-di-tert-butylphenol
Common names and synonyms:	2,6-di-tert-butylphenol
CAS number:	128-39-2
EC number:	204-884-0
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

Following eye contact

First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.

Following ingestion

Rinse mouth. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Irritates eyes and (on prolonged contact) skin. Ingestion causes irritation of mouth and stomach. (USCG, 1999)

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

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Fire Extinguishing Agents Not to Be Used: Water may be ineffective. Fire Extinguishing Agents: Dry chemical, foam, carbon dioxide (USCG, 1999)

Specific hazards arising from the chemical

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)

Special protective actions for fire-fighters

Use water spray, foam, powder, carbon dioxide.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered plastic containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered plastic containers. Carefully collect remainder. Then store and dispose of according to local regulations.

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

NO open flames. 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 in an area without drain or sewer access. Separated from food and feedstuffs. See Chemical Dangers.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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 safety goggles.

Skin protection

Protective gloves.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid.
Colour:	Light straw, crystalline solid
Odour:	no data available
Melting point/freezing point:	37 °C.
Boiling point or initial boiling point and boiling range:	253 °C. Atm. press.:Ca. 1 atm.
Flammability:	Combustible.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	Ca. 108.5 °C. Atm. press.:Ca. 101.3 kPa.
Auto-ignition temperature:	375°C
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	2.5 mg/l @ 25 deg C
Partition coefficient n-octanol/water:	log Pow = 4.5. Temperature:24 °C. Remarks:PH not reported.
Vapour pressure:	0.008 mm Hg. Temperature:20 °C. Remarks:Standard Deviation of 0.0003 mm Hg.

Density and/or relative density:	0.914 g/cm3. Temperature:20 °C.
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Reacts with acid anhydrides, acid chlorides, bases and oxidants. Attacks steel, brass and copper.

Chemical stability

no data available

Possibility of hazardous reactions

Phenols, such as DIBUTYLPHENOL, do not behave as organic alcohols, as one might guess from the presence of a hydroxyl (-OH) group in their structure. Instead, they react as weak organic acids. Phenols and cresols are much weaker as acids than common carboxylic acids (phenol has pKa = 9.88). These materials are incompatible with strong reducing substances such as hydrides, nitrides, alkali metals, and sulfides. Flammable gas (H2) is often generated, and the heat of the reaction may ignite the gas. Heat is also generated by the acid-base reaction between phenols and bases. Such heating may initiate polymerization of the organic compound. Phenols are sulfonated very readily (for example, by concentrated sulfuric acid at room temperature). The reactions generate heat. Phenols are also nitrated very rapidly, even by dilute nitric acid.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - > 5 000 mg/kg bw.

Inhalation: no data available

Dermal: no data available

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

The substance is irritating to the eyes, skin and respiratory tract.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly when dispersed.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 1.4 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 0.45 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 3.6 mg/L - 72 h.

Toxicity to microorganisms: EC50 - a mixed population of activated sewage sludge microorganisms - > 1 000 mg/L - 3 h.
Remarks:Respiration rate.

Persistence and degradability

Conversion of 1.1% of the initial concentration of 2,6-di-tert-butylphenol (50 ug) (a further 44.9% was metabolized, but not to completion)(1), 3.5%(2), and 7.7%(3) of the parent compound to CO2 by an activated sludge inoculum was reported over a 5 day time period.

Bioaccumulative potential

Chlorella, a green algae, had a measured bioaccumulation factor of 800 after exposure to 50 ug/L 2,6-di-tert-butylphenol for 24 hours(1). In fish (Golden Orfe), a bioaccumulation factor of 660 was measured following exposure to 37 ug/L 2,6-di-tert-butylphenol for 3 days(2). An estimated BCF value of 3230 was calculated for 2,6-di-tert-butylphenol(SRC), using an experimental log Kow of 4.92(3) and a recommended regression-derived equation(4). According to a recommended classification scheme(5), these BCF values indicate that bioconcentration in aquatic organisms is an important fate process(SRC).

Mobility in soil

A Koc of 3600 was measured in river sediment(1). The Koc of 2,6-di-tert-butylphenol is estimated as approximately 11,000(SRC), using an experimental log Kow of 4.92(2) and a regression-derived equation(3,SRC). According to a recommended classification scheme(4), these Koc values suggest that 2,6-di-tert-butylphenol will have slight to no mobility in soil(SRC). Following 5 days incubation, 31.9% of the initial concentration of 2,6-di-tert-butylphenol was present in the non-extractable residue fraction in sludge(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: UN2810 (For reference only, please check.)
IMDG: UN2810 (For reference only, please check.)
IATA: UN2810 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: TOXIC LIQUID, ORGANIC, N.O.S. (For reference only, please check.)
IMDG: TOXIC LIQUID, ORGANIC, N.O.S. (For reference only, please check.)
IATA: TOXIC LIQUID, ORGANIC, N.O.S. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)
IMDG: 6.1 (For reference only, please check.)
IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)
IMDG: I (For reference only, please check.)
IATA: I (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/