Chemical Safety Data Sheet MSDS / SDS

2-sec-butylphenol SDS

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

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

Product identifier

Product name: 2-sec-butylphenol

CAS: 89-72-5

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

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

uses:

Uses advised none

against:

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

Acute toxicity - Category 4, Oral Skin corrosion, Sub-category 1C

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H302 Harmful if swallowed H314 Causes severe skin burns and eye damage H318 Causes serious eye damage

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.

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

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

Response

P301+P317 IF SWALLOWED: Get medical help.

P330 Rinse mouth.

P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.

P363 Wash contaminated clothing before reuse.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P316 Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continue rinsing.

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.

Storage

P405 Store locked up.

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-sec-butylphenol
Common names and 2-sec-butylphenol

synonyms:

CAS number: 89-72-5

EC number: 201-933-8

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention.

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. Do NOT induce vomiting. Refer for medical attention.

Most important symptoms/effects, acute and delayed

Exposure Routes: inhalation, skin absorption, ingestion, skin and/or eye contact Symptoms: Irritation eyes, skin, respiratory system; skin burns Target Organs: Eyes, skin, respiratory system (NIOSH, 2016)

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

no data available

SECTION 5: Firefighting measures

Suitable extinguishing media

Fires involving this compound should be controlled with a dry chemical, carbon dioxide or halon extinguisher. (NTP, 1992)

Specific hazards arising from the chemical

This chemical is combustible. (NTP, 1992)

Special protective actions for fire-fighters

Use carbon dioxide, foam, powder.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Collect leaking and spilled liquid in sealable containers as far as possible. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations. Personal protection: chemical protection suit.

Environmental precautions

Collect leaking and spilled liquid in sealable containers as far as possible. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations. Personal protection: chemical protection suit.

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

Separated from acid anhydrides, acid chlorides, bases and food and feedstuffs.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 5 ppm as TWA; (skin)

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 face shield.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state: Liquid.

Colourless to yellowish. Colour:

no data available Odour:

9.85°C. Atm. press.:101.1 kPa. Melting

point/freezing

point:

Boiling point or 228.85°C. Atm. press.:101.1 kPa.

initial boiling point and boiling range:

Flammability: Class IIB Combustible Liquid Combustible Solid no data available

Lower and upper

explosion

limit/flammability

limit:

Flash point: 100 °C. Atm. press.:101 kPa.

Auto-ignition

320 °C. Atm. press.:>= 1 012.5 - <= 1 022.4 hPa.

temperature:

Decomposition

no data available

temperature:

no data available pH: Kinematic no data available

viscosity:

Solubility: less than 1 mg/mL at 68° F (NTP, 1992)

Partition log Pow = 3. Temperature:25 °C.;Pow = 1 000. Temperature:25 °C.

coefficient noctanol/water: Vapour pressure: 2.98 Pa. Temperature: 20 °C.

Density and/or 0.98 g/cm3. Temperature:20 °C.

relative density:

Relative vapour (air = 1): 5.2

density:

Particle no data available

characteristics:

SECTION 10: Stability and reactivity

Reactivity

Reacts with oxidants. Reacts violently with bases, acid anhydrides and acid chlorides. Attacks steel and copper and its alloys.

Chemical stability

Slightly volatile

Possibility of hazardous reactions

Phenols, such as O-SEC-BUTYLPHENOL, 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

STABILITY: This compound should be stable under normal laboratory conditions. (NTP, 1992)

Hazardous decomposition products

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male/female) - > 200 - < 2 000 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 corrosive to the eyes and skin. The vapour is irritating to the respiratory tract. Corrosive on ingestion.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Oncorhynchus mykiss (previous name: Salmo gairdneri) - > 1 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 3.7 mg/L - 48 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricomutum) - 10 mg/L - 72 h.

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

Persistence and degradability

Resting cells of a Pseudomonas strain, obtained by selective enrichment with 4-hydroxybenzoate as the sole carbon source, were able to biodegrade 2-(1-methylpropyl)phenol (oxygen uptake rate of 42 nmol O2/min/mg protein)(1). A structurally similar compound, 4-s-butylphenol (at 100 mg/L), was not biodegraded over a 2 week period using an activated sludge inoculum(2); however, a phenol-adapted yeast strain, isolated from soil, readily oxidized 4-s-butylphenol (present at 1 mmole) without a lag period(3).

Bioaccumulative potential

An estimated BCF value of 180 was calculated for 2-(1-methylpropyl)phenol(SRC), using an experimental log Kow of 3.27(1) and a recommended regression-derived equation(2). According to a recommended classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms may occur(SRC).

Mobility in soil

The Koc of 2-(1-methylpropyl)phenol is estimated as approximately 1400(SRC), using an experimental log Kow of 3.27(1) and a regression-derived equation(2,SRC). According to a recommended classification scheme(3), this estimated Koc value suggests that 2-(1-methylpropyl)phenol has low mobility in soil(SRC).

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: UN3145 (For reference only, please check.) IMDG: UN3145 (For reference only, please check.) IATA: UN3145 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ALKYLPHENOLS, LIQUID, N.O.S. (including C2-C12 homologues) (For reference only, please check.) IMDG: ALKYLPHENOLS, LIQUID, N.O.S. (including C2-C12 homologues) (For reference only, please check.) IATA: ALKYLPHENOLS, LIQUID, N.O.S. (including C2-C12 homologues) (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 8 (For reference only, please check.) IMDG: 8 (For reference only, please check.) IATA: 8 (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: No IMDG: No IATA: No

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/

Other Information

Health effects of exposure to the substance have not been investigated adequately.

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any