Chemical Safety Data Sheet MSDS / SDS

Pentachlorophenol 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:	Pentachlorophenol
CAS:	87-86-5

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

Acute toxicity - Category 3, Oral
Acute toxicity - Category 3, Dermal

Skin irritation, Category 2
Eye irritation, Category 2
Acute toxicity - Category 2, Inhalation
Specific target organ toxicity – single exposure, Category 3
Carcinogenicity, 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 Danger

Hazard statement(s)

H301 Toxic if swallowed
H311 Toxic in contact with skin
H315 Causes skin irritation
H319 Causes serious eye irritation
H330 Fatal if inhaled
H335 May cause respiratory irritation
H351 Suspected of causing cancer
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P203 Obtain, read and follow all safety instructions before use.
P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.
P332+P317 If skin irritation occurs: Get medical help.
P362+P364 Take off contaminated clothing and wash it before reuse.
P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P320 Specific treatment is urgent (see ... on this label).
P319 Get medical help if you feel unwell.
P318 IF exposed or concerned, get medical advice.
P391 Collect spillage.

Storage

P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

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:	Pentachlorophenol
Common names and synonyms:	Pentachlorophenol
CAS number:	87-86-5
EC number:	201-778-6

Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Half-upright position. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention . Wear protective gloves when administering first aid.

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 a slurry of activated charcoal in water to drink. Give one or two glasses of water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Dust or vapor irritates skin and mucous membranes, causing coughing and sneezing. Ingestion causes loss of appetite, respiratory difficulties, anesthesia, sweating, coma. Overexposure can cause death. (USCG, 1999)

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

Supportive treatment and hyperthermia control. There is no specific antidote to the poisoning; therefore treatment is supportive in nature including oxygen, fluid replacement, and most importantly, fever control. Reduce elevated body temperature by physical means. Administer sponge baths and use fans to increase evaporation. In fully conscious patients, administer cold, sugar-containing liquids by mouth as tolerated. Cooling blankets and ice packs to body surfaces may also be used. Antipyretic therapy with salicylates is strongly contraindicated as salicylates also uncouple oxidative phosphorylation. Other antipyretics are thought to be of no use because of the peripherally mediated mechanism of hyperthermia in poisoning of this nature. Neither the safety nor the effectiveness of the other antipyretics has been tested. Administer oxygen continuously by mask to minimize tissue anoxia. Unless there are manifestations of cerebral or pulmonary edema or of inadequate renal function, administer intravenous fluids to restore hydration and support physiologic mechanisms for heat loss and toxicant disposition. Monitor serum electrolytes, adjusting IV infusions to stabilize electrolyte concentrations. Follow urine contents of albumin and cells, and keep an accurate hourly record of intake/output to forestall fluid overload if renal function declines. Caution: In the presence of cerebral edema and/or impaired

renal function, intravenous fluids must be administered very cautiously to avoid increased intracranial pressure and pulmonary edema. Central monitoring of venous and pulmonary wedge pressures may be indicated. Such critically ill patients should be treated in an intensive care unit.

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Extinguish fire using agent suitable for type of surrounding fire. Material itself does not burn or burns with difficulty.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Generates toxic and irritating vapors. (USCG, 1999)

Special protective actions for fire-fighters

In case of fire in the surroundings, use appropriate extinguishing media.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: chemical protection suit and filter respirator for organic gases and particulates adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: chemical protection suit and filter respirator for organic gases and particulates adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Shovel into suitable dry container.

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

Provision to contain effluent from fire extinguishing. Separated from strong oxidants and food and feedstuffs. Keep in a well-ventilated room.Where possible, automatically transfer material from drums or other storage containers to process containers. Sources of ignition such as smoking and open flames are prohibited where this chemical is handled, used, or stored. Metal containers involving the transfer of this chemical should be grounded and bonded. A regulated, marked area should be established where this chemical is handled, used or stored ...

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.5 mg/m3, as TWA; 1 mg/m3 as STEL; (skin); A3 (confirmed animal carcinogen with unknown relevance to humans); BEI issued.MAK: skin absorption (H); carcinogen category: 2

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, face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Pentachlorophenol is a white crystalline solid. Slightly soluble in water. Noncombustible. Toxic by inhalation, ingestion, and skin absorption. Used as a fungicide and as a wood preservative.
Colour:	White monoclinic, crystalline solid
Odour:	Phenolic odor
Melting point/freezing point:	165-180°C
Boiling point or initial boiling point and boiling range:	310°C
Flammability:	Noncombustible Solid
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	133.7°C
Auto-ignition temperature:	Not flammable (USCG, 1999)
Decomposition temperature:	309°C
pH:	no data available

Kinematic viscosity:	no data available
Solubility:	less than 1 mg/mL at 68° F (NTP, 1992)
Partition coefficient n-octanol/water:	log Kow = 5.12
Vapour pressure:	40 mm Hg (211.2 °C)
Density and/or relative density:	1.97
Relative vapour density:	9.2 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes above 200°C . This produces toxic and corrosive fumes including dioxins. Reacts violently with strong oxidants. Decomposes on heating. This produces toxic and corrosive fumes including hydrogen chloride and dioxins. Reacts with strong oxidants. This generates fire and explosion hazard.

Chemical stability

Stable; prolonged heating above 200 deg C produces traces of octachlorodibenzo-para-dioxin.

Possibility of hazardous reactions

Not combustible but if involved in a fire decomposes to produce hydrogen chloride and other irritants and toxic gases. May be in hydrocarbon solution.PENTACHLOROPHENOL may react with strong oxidizing agents. Incompatible with strong bases, acid chlorides and acid anhydrides. Forms salts with alkaline metals. Solutions in oil cause natural rubber to deteriorate, but synthetic rubber may be used in equipment and for protective clothing (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Contact with strong oxidizers may cause fires or explosions.

Hazardous decomposition products

Hydrogen chloride, chlorinated phenols, and carbon monoxide may be released upon decomposition.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat male oral 146 mg/kg

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

Evaluation: There is limited evidence in humans for the carcinogenicity of combined exposures to polychlorophenols and their sodium salts. ... There is sufficient evidence in experimental animals for the carcinogenicity of pentachlorophenol. Overall evaluation: Combined exposures to polychlorophenols or to their sodium salts are possibly carcinogenic to humans (Group 2B). Polychlorophenols & sodium salts

Reproductive toxicity

One study reported that 22 out of 90 women with histories of spontaneous abortions, unexplained infertility, or menstrual disorders were found to have elevated blood levels of pentachlorophenol and/or lindane. However, a direct causal relationship with pentachlorophenol exposure cannot be inferred from this study due to the presence of lindane in the blood and other possible confounding factors. Oral animal studies suggest that exposure to pentachlorophenol decreases the survival of the offspring in rats. Other oral animal studies have found evidence that pentachlorophenol produces maternal toxicity (depressed maternal body weight), but does not cause birth defects.

STOT-single exposure

The substance is irritating to the eyes, skin and respiratory tract. The substance may cause effects on the cardiovascular system. This may result in cardiac disorders and heart failure.

STOT-repeated exposure

The substance may have effects on the central nervous system, kidneys, liver, lungs, immune system and thyroid. This substance is possibly carcinogenic to humans. Animal tests show that this substance possibly causes toxicity to human reproduction or development.

Aspiration hazard

Evaporation at 20°C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: Brachydanio rerio (Zebra fish); Conditions: flow through bioassay, 25 deg C; Concentration: 1.24 mg/L for 48 hr; 1.13 mg/L for 96 hr; 1.08 mg/L for 10 days

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater, static, > or =20 deg C; Concentration: 0.544 umol/L for 48 hr; Effect: behavior, equilibrium />98% purity

Toxicity to algae: EC50; Species: Pseudokirchneriella subcapitata (Green algae, log growth phase); Conditions: freshwater, static, 23 deg C; Concentration: 240 ug/L for 72 hr; Effect: decreased population abundance /formulation

Toxicity to microorganisms: no data available

Persistence and degradability

Screening biodegradability tests give conflicting results(1-7); pentachlorophenol does biodegrade but may require several weeks for acclimation(3-7). Using an acclimated pentachlorophenol-degrading culture, half-lives of 85 (lag time of 27 hours) and 420 (lag time of 220 hours) hours were reported for aerobic and anaerobic conditions, respectively(8). Pentachlorophenol, present at 100 mg/L, reached 1% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(9). Acclimation of microbial communities to pentachlorophenol appears to increase tolerance to pentachlorophenol and/or select for pentachlorophenol-tolerant microorganisms(10). Pentachlorophenol, at an initial concn of 300-500 ug/L, had a half-life of 2.6 days using a sludge inoculum(11). At this concentration, no lag phase was seen(11).

Bioaccumulative potential

BCF values of 776 in fathead minnow(1), 251-5370 in rainbow trout(2,3), 5-50 in sheepshead minnows(4), 295 in mosquito fish(5); 708(6), 960(7), and 977(8) in zebra fish, and 417 in golden orfe(6) have been reported. The accumulation increased with temperature in golden orfe and decreased with temperature in zebra fish(6). BCF values of 39-198 and 45-224 were measured in an 8-week carp study with pentachlorophenol concns of 30 and 3 ug/L, respectively(9). BCF values of 214 in Jordanella floridae and 380-1698 in Oryzias latipes were reported for pentachlorophenol(8). A BCF value of 13 was measured in bluegill muscle in an 8-day study(10). According to a classification scheme(11), these BCF values suggest that bioconcentration in aquatic organisms is low to very high(SRC), with the value being greatly influenced by environmental pH(12).

Mobility in soil

Koc values for pentachlorophenol of 2285 (pH 4.9), 4267 (pH 5.0), 6224 (pH 5.9), 3684 (pH 4.6), 121681 (pH 3.5), 121810 (pH 3.9), 97471 (pH 3.7), 1586 (pH 5.0), 4109 (pH 5.1), 4009 (pH 5.5), 123563 (pH 3.5) have been reported(1). According to a classification scheme(2), these Koc values indicate that pentachlorophenol is expected to have slight to no mobility in soil(SRC). Freundlich isotherm coefficients were determined to be 5 (silty sand soil), 5 (aquifer), and 3 (marine sediment)(9). A log Koc of 3.16 was observed in sediment of the Yangtse River in China(10). Since pentachlorophenol has a pKa of 4.70(3), its adsorptivity will be strongly dependent on pH. The Freundlich adsorption constant for 6 Dutch soils are (soil (% organic carbon, pH) log KF, 1/N): humic sand (1.7%, 3.4) 2.2, 0.9; humic sand (2.2%, 4.9) 2.2, 0.9; humic-rich sand (3.2%, 4.7) 2.6, 1.0; peat (29.8%, 4.6) 3.3, 0.8; light loam (0.9%, 7.5) 1.1, 0.9; heavy loam (1.7%, 7.1) 1.5, 0.8(4). For loam soil where pH >pKa, significant contribution from the phenolate ion can be expected. The Koc values for the total dissociated phenol was calculated to be 1250 and 1800 for light and heavy loam, respectively, while for the undissociated species, the Koc is 25,000(5). The fraction of pentachlorophenol which is sorbed decreases linearly with pH to a pH 6; above pH 6, significant adsorption of the anion again occurs, contributing as much as 20% of the total adsorption effect at pH 8(4). K values for a Bjuv clay (organic carbon 12%) and an aquifer soil (organic carbon 0.02%) were 433 and 86 at pH 3.0, respectively, and 167 and 50 at pH 6.5, respectively(4). K values for a bentonite clay of 72 and 34 were measured at pH 3.0 and 6.5, respectively(4). The nonionized form of pentachlorophenol had a K value of 3.63 mL/g in a sandy aquifer material (organic C 0.13%) (Koc 2792)(6). K values measured at pH 7 for a Guishan sandy loam (organic carbon 1.4%) and a Shulin clay loam (organic carbon 2.0%) were 2.56 (Koc 183) and 7.03 (Koc 352), respectively(7). The Koc for pentachlorophenol was measured for five soils (foc from 0.07 to 2.96%; 3 sands, 1 loamy sand, 1 loam)(8). At pH 4, 7, and 10, the Koc values ranged from 10091-40120 (avg 19675), 178-1956 (avg 651), and 126-942 (avg 501), respectively(8).

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: UN2761 (For reference only, please check.)
IMDG: UN2761 (For reference only, please check.)
IATA: UN2761 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: ORGANOCHLORINE PESTICIDE, SOLID, TOXIC (For reference only, please check.)
IMDG: ORGANOCHLORINE PESTICIDE, SOLID, TOXIC (For reference only, please check.)
IATA: ORGANOCHLORINE PESTICIDE, SOLID, TOXIC (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

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not 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

The commercial product may contain very toxic impurities (dioxins).The odour warning when the exposure limit value is exceeded is insufficient.

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