SAFETY DATA SHEET

Updated on 26/09/2024

1. Material Identification

Product Name : Pentachlorophenol
Catalog Number : io-2814
CAS Number : 87-86-5
Identified uses : Laboratory chemicals, manufacture of chemical compounds
Company : Ionz

>> R&D Use only

2. Hazards Identification

GHS Classification:

Flammable liquid (category 2)
Acute toxicity, oral (Category 3)
Acute toxicity, dermal (Category 3)
Acute toxicity, inhalation (Category 3)
Specific target organ toxicity, single exposure (Category 1)

Pictogram(s)

GHS Hazard Statements

>> H300 (33.3%): Fatal if swallowed [Danger Acute toxicity, oral]

>> H301 (66.7%): Toxic if swallowed [Danger Acute toxicity, oral]

>> H310 (33.3%): Fatal in contact with skin [Danger Acute toxicity, dermal]

>> H311 (66.7%): Toxic in contact with skin [Danger Acute toxicity, dermal]

>> H315 (100%): Causes skin irritation [Warning Skin corrosion/irritation]

>> H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation]

>> H330 (100%): Fatal if inhaled [Danger Acute toxicity, inhalation]

>> H335 (66.7%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]

>> H351 (100%): Suspected of causing cancer [Warning Carcinogenicity]

>> H400 (100%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H410 (66.7%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

>> H413 (33.3%): May cause long lasting harmful effects to aquatic life [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P203, P260, P261, P262, P264, P264+P265, P270, P271, P273, P280, P284, P301+P316, P302+P352, P304+P340, P305+P351+P338, P316, P318, P319, P320, P321, P330, P332+P317, P337+P317, P361+P364, P362+P364, P391, P403+P233, P405, and P501

NFPA 704 Diamond

NFPA Health Rating

>> 3 - Materials that, under emergency conditions, can cause serious or permanent injury.

NFPA Fire Rating

>> 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA Instability Rating

>> 0 - Materials that in themselves are normally stable, even under fire conditions.

Health Hazards:

>> 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)

ERG 2024, Guide 154 (Pentachlorophenol)

>> TOXIC and/or CORROSIVE; inhalation, ingestion or skin contact with material may cause severe injury or death.

>> Contact with molten substance may cause severe burns to skin and eyes.

>> Avoid any skin contact.

>> Fire may produce irritating, corrosive and/or toxic gases.

>> Runoff from fire control or dilution water may be corrosive and/or toxic and cause environmental contamination.

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

ERG 2024, Guide 154 (Pentachlorophenol)

>> Non-combustible, substance itself does not burn but may decompose upon heating to produce corrosive and/or toxic fumes.

>> Some are oxidizers and may ignite combustibles (wood, paper, oil, clothing, etc.).

>> Corrosives in contact with metals may evolve flammable hydrogen gas.

>> Containers may explode when heated.

>> For electric vehicles or equipment, GUIDE 147 (lithium ion or sodium ion batteries) or GUIDE 138 (sodium batteries) should also be consulted.

>> Not combustible. Liquid formulations containing organic solvents may be flammable.

3. Composition/Information On Ingredients

Chemical name : Pentachlorophenol
CAS Number : 87-86-5
Molecular Formula : C6HCl5O
Molecular Weight : 266.3000 g/mol

4. First Aid Measures

First Aid:

>> EYES: First check the victim for contact lenses and remove if present. Flush victim's eyes with water or normal saline solution for 20 to 30 minutes while simultaneously calling a hospital or poison control center. Do not put any ointments, oils, or medication in the victim's eyes without specific instructions from a physician. IMMEDIATELY transport the victim after flushing eyes to a hospital even if no symptoms (such as redness or irritation) develop.

>> SKIN: IMMEDIATELY flood affected skin with water while removing and isolating all contaminated clothing. Gently wash all affected skin areas thoroughly with soap and water. IMMEDIATELY call a hospital or poison control center even if no

symptoms (such as redness or irritation) develop. IMMEDIATELY transport the victim to a hospital for treatment after washing the affected areas.

>> INHALATION: IMMEDIATELY leave the contaminated area; take deep breaths of fresh air. IMMEDIATELY call a physician and be prepared to transport the victim to a hospital even if no symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop. Provide proper respiratory protection to rescuers entering an unknown atmosphere. Whenever possible, Self-Contained Breathing Apparatus (SCBA) should be used; if not available, use a level of protection greater than or equal to that advised under Protective Clothing.

>> INGESTION: DO NOT INDUCE VOMITING. Phenols are very toxic poisons AND corrosive and irritating, so that inducing vomiting may make medical problems worse. IMMEDIATELY call a hospital or poison control center and locate activated charcoal, egg whites, or milk in case the medical advisor recommends administering one of them. If advice from a physician is not readily available and the victim is conscious and not convulsing, give the victim a glass of activated charcoal slurry in water or, if this is not available, a glass of milk, or beaten egg whites and IMMEDIATELY transport victim to a hospital. If the victim is convulsing or unconscious, do not give anything by mouth, assure that the victim's airway is open and lay the victim on his/her side with the head lower than the body. DO NOT INDUCE VOMITING. IMMEDIATELY transport the victim to a hospital.

>> OTHER: Since this chemical is a known or suspected carcinogen you should contact a physician for advice regarding the possible long term health effects and potential recommendation for medical monitoring. Recommendations from the physician will depend upon the specific compound, its chemical, physical and toxicity properties, the exposure level, length of exposure, and the route of exposure. (NTP, 1992)

ERG 2024, Guide 154 (Pentachlorophenol)

>> General First Aid:

>> Call 911 or emergency medical service.

>> Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and avoid contamination.

>> Move victim to fresh air if it can be done safely.

>> Administer oxygen if breathing is difficult.

>> If victim is not breathing:

>> DO NOT perform mouth-to-mouth resuscitation; the victim may have ingestedor inhaled the substance.

>> If equipped and pulse detected, wash face and mouth, then give artificial respiration using a proper respiratory medical device (bag-valve mask, pocket mask equipped with a one-way valve or other device).

>> If no pulse detected or no respiratory medical device available, provide continuouscompressions. Conduct a pulse check every two minutes or monitor for any signs of spontaneous respirations.

>> Remove and isolate contaminated clothing and shoes.

>> For minor skin contact, avoid spreading material on unaffected skin.

>> In case of contact with substance, remove immediately by flushing skin or eyes with running water for at least 20 minutes.

>> For severe burns, immediate medical attention is required.

>> Effects of exposure (inhalation, ingestion, or skin contact) to substance may be delayed.

>> Keep victim calm and warm.

>> Keep victim under observation.

>> For further assistance, contact your local Poison Control Center.

>> Note: Basic Life Support (BLS) and Advanced Life Support (ALS) should be done by trained professionals.

>> Specific First Aid:

>> For corrosives, in case of contact, immediately flush skin or eyes with running water for at least 30 minutes. Additional flushing may be required.

>> In Canada, an Emergency Response Assistance Plan (ERAP) may be required for this product. Please consult the shipping paper and/or the "ERAP" section.

First Aid Measures

Inhalation First Aid

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

Skin First Aid

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

Eye First Aid

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

Ingestion First Aid

>> 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 .

5. Fire Fighting Measures

>> Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

>> SMALL FIRE: Dry chemical, CO2 or water spray.

>> LARGE FIRE: Dry chemical, CO2, alcohol-resistant foam or water spray. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal.

>> FIRE INVOLVING TANKS, RAIL TANK CARS OR HIGHWAY TANKS: Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles. Do not get water inside containers. Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks in direct contact with flames. (ERG, 2024)

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

6. Accidental Release Measures

Isolation and Evacuation:

Isolation and evacuation measures to take when a large amount of this chemical is accidentally released in an emergency.

>> Excerpt from ERG Guide 154 [Substances - Toxic and/or Corrosive (Non-Combustible)]:

>> IMMEDIATE PRECAUTIONARY MEASURE: Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

>> SPILL: Increase the immediate precautionary measure distance, in the downwind direction, as necessary.

>> FIRE: If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions. (ERG, 2024)

Evacuation: ERG 2024, Guide 154 (Pentachlorophenol)

>> Immediate precautionary measure

>> Isolate spill or leak area in all directions for at least 50 meters (150 feet) for liquids and at least 25 meters (75 feet) for solids.

>> Spill

>> For non-highlighted materials: increase the immediate precautionary measure distance, in the downwind direction, as necessary.

>> Fire

>> If tank, rail tank car or highway tank is involved in a fire, ISOLATE for 800 meters (1/2 mile) in all directions; also, consider initial evacuation for 800 meters (1/2 mile) in all directions.

Spillage Disposal:

Methods for containment and safety measures to protect workers dealing with a spillage of this chemical.

>> 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.

Accidental Release Measures

Public Safety: ERG 2024, Guide 154 (Pentachlorophenol)

>> CALL 911. Then call emergency response telephone number on shipping paper. If shipping paper not available or no answer, refer to appropriate telephone number listed on the inside back cover.

>> Keep unauthorized personnel away.

>> Stay upwind, uphill and/or upstream.

>> Ventilate closed spaces before entering, but only if properly trained and equipped.

Spill or Leak: ERG 2024, Guide 154 (Pentachlorophenol)

>> ELIMINATE all ignition sources (no smoking, flares, sparks or flames) from immediate area.

>> Do not touch damaged containers or spilled material unless wearing appropriate protective clothing.

>> Stop leak if you can do it without risk.

>> Prevent entry into waterways, sewers, basements or confined areas.

>> Absorb or cover with dry earth, sand or other non-combustible material and transfer to containers.

>> DO NOT GET WATER INSIDE CONTAINERS.

7. Handling And Storage

Safe Storage:

>> Provision to contain effluent from fire extinguishing. Separated from strong oxidants and food and feedstuffs. Keep in a well-ventilated room.

Storage Conditions:

>> 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 ...

8. Exposure Control/ Personal Protection

REL-TWA (Time Weighted Average)

>> 0.5 mg/m³

>> TWA 0.5 mg/m3 [skin]

>> 0.5 [mg/m3]

PEL-TWA (8-Hour Time Weighted Average)

>> 0.5 mg/m³

>> 0.5 [mg/m3], inhalable fraction and vapor

TLV-STEL

>> 1.0 [mg/m3], inhalable fraction and vapor

>> 0.5 mg/m

TLV-TWA (Time Weighted Average)

>> 0.5 mg/m³ (inhalable fraction and vapor)[2013]

TLV-STEL (Short Term Exposure Limit)

>> 1 mg/m³ (inhalable fraction and vapor) [2013]

MAK (Maximale Arbeitsplatz Konzentration)

>> skin absorption (H); carcinogen category: 2

Emergency Response: ERG 2024, Guide 154 (Pentachlorophenol)

>> Small Fire

>> Dry chemical, CO2 or water spray.

>> Large Fire

>> Dry chemical, CO2, alcohol-resistant foam or water spray.

>> If it can be done safely, move undamaged containers away from the area around the fire.

>> Dike runoff from fire control for later disposal.

>> Fire Involving Tanks, Rail Tank Cars or Highway Tanks

>> Fight fire from maximum distance or use unmanned master stream devices or monitor nozzles.

>> Do not get water inside containers.

>> Cool containers with flooding quantities of water until well after fire is out.

>> Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank.

>> ALWAYS stay away from tanks in direct contact with flames.

Inhalation Risk:

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

Effects of Short Term 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.

Effects of Long Term 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.

Exposure Prevention

>> PREVENT DISPERSION OF DUST! STRICT HYGIENE! AVOID EXPOSURE OF (PREGNANT) WOMEN! AVOID ALL CONTACT! IN ALL CASES CONSULT A DOCTOR!

Inhalation Prevention

>> Use local exhaust or breathing protection.

Skin Prevention

>> Protective gloves. Protective clothing.

Eye Prevention

>> Wear safety goggles, face shield or eye protection in combination with breathing protection.

Ingestion Prevention

>> Do not eat, drink, or smoke during work. Wash hands before eating.

Exposure Control and Personal Protection

Protective Clothing: ERG 2024, Guide 154 (Pentachlorophenol)

>> Wear positive pressure self-contained breathing apparatus (SCBA).

>> Wear chemical protective clothing that is specifically recommended by the manufacturer when there is NO RISK OF FIRE.

>> Structural firefighters' protective clothing provides thermal protection but only limited chemical protection.

Exposure Summary

>> Biological Exposure Indices (BEI) [ACGIH] - PCP in urine (with hydrolysis) prior to last shift of workweek: Nq (Biological monitoring should be considered for this compound based on the review; however, a specific BEI could not be determined due to insufficient data.) [TLVs and BEIs]

>> TIH (Toxic Inhalation Hazard) - Term used to describe gases and volatile liquids that are toxic when inhaled. Some are TIH materials themselves, e.g., chlorine, and some release TIH gases when spilled in water, e.g., chlorosilanes. [ERG 2016].

9. Physical And Chemical Properties

Molecular Weight:

>> 266.3

Exact Mass:

>> 265.844053

Physical Description:

>> Pentachlorophenol appears as 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.

>> WHITE CRYSTALS OR SOLID IN VARIOUS FORMS WITH CHARACTERISTIC ODOUR.

Color/Form:

>> White monoclinic, crystalline solid

Odor:

>> Phenolic odor

Taste:

The sensation of flavor perceived in the mouth and throat on contact with a substance.

>> Taste threshold of 30 ug/L

Boiling Point:

>> 588 to 590 °F at 760 mmHg (with decomposition) (NTP, 1992)

Melting Point:

>> 376 °F (NTP, 1992)

>> 191 °C

Solubility:

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

>> Solubility in water, g/100ml at 20 °C: 0.001

Density:

>> 1.98 at 59 °F (USCG, 1999) - Denser than water; will sink

>> 1.98 g/cm³

Vapor Density:

>> 9.2 (NTP, 1992) - Heavier than air; will sink (Relative to Air)

>> Relative vapor density (air = 1): 9.2

Vapor Pressure:

>> 0.00011 mmHg at 68 °F ; 40 mmHg at 412.2 °F (NTP, 1992)

>> Vapor pressure, Pa at 20 °C: 0.02

LogP:

>> log Kow = 5.12

>> 5.01

Stability/Shelf Life:

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

Autoignition Temperature:

>> Not flammable (USCG, 1999)

Decomposition:

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

>> 309 °C

Corrosivity:

The ability of a chemical to damage or destroy other substances when it comes into contact.

>> Noncorrosive in absence of moisture

Heat of Vaporization:

>> 16,742.6 gcal/gmole

Ionization Efficiency:

The ratio of the number of ions formed to the number of electrons or photons used in an ionization process.

Ionization mode

>> Negative

logIE

>> 1.97

pH

>> 10.5

Instrument

>> Agilent XCT

Ion source

>> Electrospray ionization

Additive

>> ammonia (10nM)

Organic modifier

>> MeCN (80%)

Reference

>> DOI:10.1021/acs.analchem.7b00595

Odor Threshold:

>> Odor thresholds for PCP soln at 30 deg and 60 °C were 857 and 12,000 ug/l, respectively.

Dissociation Constants:

>> pKa = 4.70

Collision Cross Section:

Collision cross section (CCS) represents the effective area for the interaction between an individual ion and the neutral gas through which it is traveling (e.g., in ion mobility spectrometry (IMS) experiments). It quantifies the probability of a collision taking place between two or more particles.

>> 135.93 Å² [M-H]-

10. Stability And Reactivity

>> Slightly soluble in water.

11. Toxicological Information

Toxicity Summary:

>> Pentachlorophenol is a cholinesterase or acetylcholinesterase (AChE) inhibitor. A cholinesterase inhibitor (or 'anticholinesterase') suppresses the action of acetylcholinesterase. Because of its essential function, chemicals that interfere with the action of acetylcholinesterase are potent neurotoxins, causing excessive salivation and eye-watering in low doses, followed by muscle spasms and ultimately death. Nerve gases and many substances used in insecticides have been shown to act by binding a serine in the active site of acetylcholine esterase, inhibiting the enzyme completely. Acetylcholine esterase breaks down the neurotransmitter acetylcholine, which is released at nerve and muscle junctions, in order to allow the muscle or organ to relax. The result of acetylcholine esterase inhibition is that acetylcholine builds up and continues to act so that any nerve impulses are continually transmitted and muscle

contractions do not stop. Among the most common acetylcholinesterase inhibitors are phosphorus-based compounds, which are designed to bind to the active site of the enzyme. The structural requirements are a phosphorus atom bearing two lipophilic groups, a leaving group (such as a halide or thiocyanate), and a terminal oxygen.

USGS Health-Based Screening Levels for Evaluating Water-Quality:

This section provides the USGS Health-Based Screening Levels for Evaluating Water-Quality data.

Chemical

>> Pentachlorophenol

MCL (Maximum Contaminant Levels)[μg/L]

>> 1

Reference

>> Smith, C.D. and Nowell, L.H., 2024. Health-Based Screening Levels for evaluating water-quality data (3rd ed.). DOI:10.5066/F71C1TWP

Evidence for Carcinogenicity:

Evidence that this chemical does or may cause cancer. The information here is collected from various sources by the Hazardous Substances Data Bank (HSDB).

>> 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/

Carcinogen Classification:

This section provides the International Agency for Research on Cancer (IARC) Carcinogenic Classification and related monograph links. In the IARC Carcinogenic classification, chemicals are categorized into four groups: Group 1 (carcinogenic to humans), Group 2A (probably carcinogenic to humans), Group 2B (possibly carcinogenic to humans), and Group 3 (not classifiable as to its carcinogenicity to humans).

>> 2B, possibly carcinogenic to humans. (L135)

Health Effects:

>> Acute exposure to cholinesterase inhibitors can cause a cholinergic crisis characterized by severe nausea/vomiting, salivation, sweating, bradycardia, hypotension, collapse, and convulsions. Increasing muscle weakness is a possibility and may result in death if respiratory muscles are involved. Accumulation of ACh at motor nerves causes overstimulation of nicotinic expression at the neuromuscular junction. When this occurs symptoms such as muscle weakness, fatigue, muscle cramps, fasciculation, and paralysis can be seen. When there is an accumulation of ACh at autonomic ganglia this causes overstimulation of nicotinic expression in the sympathetic system. Symptoms associated with this are hypertension, and hypoglycemia. Overstimulation of nicotinic acetylcholine receptors in the central nervous system, due to accumulation of ACh, results in anxiety, headache, convulsions, ataxia, depression of respiration and circulation, tremor, general weakness, and potentially coma. When there is expression of muscarinic overstimulation due to excess acetylcholine at muscarinic acetylcholine receptors symptoms of visual disturbances, tightness in chest, wheezing due to bronchoconstriction, increased bronchial secretions, increased salivation, lacrimation, sweating, peristalsis, and urination can occur. Certain reproductive effects in fertility, growth, and development for males and females have been linked specifically to organophosphate pesticide exposure. Most of the research on reproductive effects has been conducted on farmers working with pesticides and insecticdes in rural areas. In females menstrual cycle disturbances, longer pregnancies, spontaneous abortions, stillbirths, and some developmental effects in offspring have been linked to organophosphate pesticide exposure. Prenatal exposure has been linked to impaired fetal growth and development. Neurotoxic effects have also been linked to poisoning with OP pesticides causing four neurotoxic effects in humans: cholinergic syndrome, intermediate syndrome, organophosphate-induced delayed polyneuropathy (OPIDP), and chronic organophosphate-induced neuropsychiatric disorder (COPIND). These syndromes result after acute and chronic exposure to OP pesticides.

Exposure Routes:

>> The substance can be absorbed into the body by inhalation, through the skin and by ingestion.

>> inhalation, skin absorption, ingestion, skin and/or eye contact

Inhalation Exposure

>> Cough. Dizziness. Drowsiness. Headache. Fever. Laboured breathing. Sore throat.

Skin Exposure

>> MAY BE ABSORBED! Redness. Blisters. Further see Inhalation.

Eye Exposure

>> Redness. Pain.

Ingestion Exposure

>> Abdominal cramps. Diarrhoea. Nausea. Unconsciousness. Vomiting. Weakness. Further see Inhalation.

>> irritation eyes, nose, throat; sneezing, cough; lassitude (weakness, exhaustion), anorexia, weight loss; sweating; headache, dizziness; nausea, vomiting; dyspnea (breathing difficulty), chest pain; high fever; dermatitis

Target Organs:

Organs that are affected by exposure to this chemical. Information in this section reflects human data unless otherwise noted.

>> Cancer, Developmental (effects during periods when organs are developing) , Hepatic (Liver)

>> Hepatic

Cancer Sites:

The site in which cancer develops due to exposure to this compound. Cancers are casually referred to based on their primary sites (e.g., skin, lung, breasts, prostate, colon and rectum).

>> Endocrine

>> Hepatic

Adverse Effects:

An adverse effect is an undesired harmful effect resulting from a medical treatment or other intervention.

>> Occupational hepatotoxin - Secondary hepatotoxins: the potential for toxic effect in the occupational setting is based on cases of poisoning by human ingestion or animal experimentation.

>> Nephrotoxin - The chemical is potentially toxic to the kidneys in the occupational setting.

>> Other Poison - Uncoupler

>> Dermatotoxin - Chloracne.

>> IARC Carcinogen - Class 1: International Agency for Research on Cancer classifies chemicals as established human carcinogens.

>> NTP Carcinogen - Reasonably anticipated to be a human carcinogen.

>> ACGIH Carcinogen - Confirmed Animal.

Toxicity Data:

>> LD50: 27 mg/kg (Oral, Rat) (T26) LD50: 96 mg/kg (Dermal, Rat) (T26) LD50: 56 mg/kg (Intraperitoneal, Rat) (T26) LD50: 58 mg/kg (Subcutaneous, Rat) (T26)

Minimum Risk Level:

The minimal risk level (MRL) is an estimate of the amount of a chemical a person can eat, drink, or breathe each day without a detectable risk to health

>> Acute Oral: 0.005 mg/kg/day (L134) Intermediate Oral: 0.001 mg/kg/day (L134) Chronic Oral: 0.001 mg/kg/day (L134)

Treatment:

Treatment when exposed to toxin

>> If the compound has been ingested, rapid gastric lavage should be performed using 5% sodium bicarbonate. For skin contact, the skin should be washed with soap and water. If the compound has entered the eyes, they should be washed with large quantities of isotonic saline or water. In serious cases, atropine and/or pralidoxime should be administered. Anti-cholinergic drugs work to counteract the effects of excess acetylcholine and reactivate AChE. Atropine can be used as an antidote in conjunction with pralidoxime or other pyridinium oximes (such as trimedoxime or obidoxime), though the use of '-oximes' has been found to be of no benefit, or possibly harmful, in at least two meta-analyses. Atropine is a muscarinic antagonist, and thus blocks the action of acetylcholine peripherally.

Interactions:

>> Investigation of the toxicological effects of pentachlorophenol (PCP) and bisphenol A (BPA) alone and in combination was carried out following the method of the early life stage (ELS) test on zebrafish embryos. Both chemicals revealed lethal and sub-lethal effects, such as no blood flow, cardiac edema, delayed hatching, and tail malformations. According to their median effective concentrations (EC(50) values) in the single exposure, the toxic level of PCP was about two orders of magnitude higher than that of BPA. Result of the joint action modes varied depending on different endpoints. Synergistic action was observed based on the endpoint of 24 hr mortality and antagonistic effect displayed based on the endpoint of 72 hr cardiac edema. It was also found that the toxicity of PCP would be enhanced with the addition of BPA even below its no observed effect concentration (NOEC) level at the endpoint of 32 hr with no blood flow, and the level of the increase was influenced by the toxic unit (TU) ratio.

Antidote and Emergency Treatment:

>> 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.

Human Toxicity Excerpts:

>> /HUMAN EXPOSURE STUDIES/ Dust and mist concn greater than 1.0 mg/cu m resulted in painful irritation of upper respiratory tract in persons not previously exposed to pentachlorophenol. Violent sneezing and coughing accompanied exposure. Conditioned persons tolerated concn up to 2.4 mg/cu m.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ It is generally agreed that the symptoms and signs of acute chlorophenol toxicity result from the effects of the chlorophenol molecule itself, rather than from the microcontaminants. Chlorophenol rapidly causes hyperthermia, profuse sweating and early death. These signs are not observed in animals exposed only to PCDD and PCDF.

Non-Human Toxicity Values:

>> LD50 Rat male oral 146 mg/kg

National Toxicology Program Studies:

Reports from the National Toxicology Program, an interagency program supported by three government agencies (NIH, FDA, and CDC) within the Department of Health and Human Services. This program plays a critical role in generating, interpreting, and sharing toxicological information about chemicals of public health concerns.

>> Carcinogenicity bioassays were conducted utilizing 0, 100, or 200 ppm technical grade pentachlorophenol or 0, 100, 200, or 600 ppm (Dowicide EC-7, a technical grade formulation) fed to groups of 50 male and 50 female /B6C3F1 mice. ... Under the conditions of these two yr studies, there was clear evidence of carcinogenic activity for male B6C3F1 mice fed diets containing technical grade pentachlorophenol, as shown by increased incidences of adrenal medullary and hepatocellular neoplasms. There was some evidence of carcinogenic activity for female B6C3F1 mice exposed to technical grade pentachlorophenol, as shown by increased incidences of hemangiosarcomas and hepatocellular carcinomas. /Also/, there was clear evidence of carcinogenic activity for male B6C3F1 mice exposed to pentachlorophenol, EC-7, as shown by increased incidences of adrenal medullary and hepatocellular neoplasms. There was clear evidence of carcinogenic activity for female B6C3F1 mice exposed to pentachlorophenol, EC-7, as shown by increased incidences of adrenal medullary and hepatocellular neoplasms and hemangiosarcomas.

Populations at Special Risk:

>> Individuals suffering from kidney and liver diseases ... should /be protected from/ occupational exposure.

12. Ecological Information

Resident Soil (mg/kg)

>> 1.00e+00

Industrial Soil (mg/kg)

>> 4.00e+00

Resident Air (ug/m3)

>> 5.50e-01

Industrial Air (ug/m3)

>> 2.40e+00

Tapwater (ug/L)

>> 4.10e-02

MCL (ug/L)

>> 1.00e+00

Risk-based SSL (mg/kg)

>> 5.7e-05

MCL-based SSL (mg/kg)

>> 1.40e-03

Oral Slope Factor (mg/kg-day)-1

>> 4.00e-01

Inhalation Unit Risk (ug/m3)-1

>> 5.1e-06

Chronic Oral Reference Dose (mg/kg-day)

>> 5.00e-03

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Fraction of Contaminant Absorbed Dermally from Soil

>> 0.25

ICSC Environmental Data:

>> The substance is very toxic to aquatic organisms. The substance may cause long-term effects in the aquatic environment. This substance does enter the environment under normal use. Great care, however, should be taken to avoid any additional release, for example through inappropriate disposal.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SOIL: Soil samples from four sites near a pentachlorophenol-production facility in Switzerland contained 25 to 140 ug/kg (dry weight) at depths of 0-10 cm and 33-184 ug/kg at 20-30 cm(1). Soil from Finnish sawmills was heavily contaminated with up to 45.6 mg/kg at 0-5 cm depth near the treatment basin and up to 0.14 mg/kg in the area for storing treated wood. The background level was 0.012 mg/kg. Avg pentachlorophenol levels in soil samples at 2.5, 30.5, and 152.5 cm from poles treated with pentachlorophenol were 658, 3.4, and 0.26 mg/kg, respectively(1). Abandoned sawmill site near a wood-preserving site in Finland - 390 ppm(2).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> Pentachlorophenol was detected in New Brunswick, Canada fish at 0.5-4 ppb collected in the fall of 1972 and in white shark liver at 10.8 ppb, collected in 1971(1). Pentachlorophenol was detected, not quantified in composite fish samples from Wabash R, IN(2). Pentachlorophenol has been detected in fish at concns ranging between 0.35-26 mg/kg(3). Flounder, killifish, shrimp, crab and squid from San Loui Pas, West Galveston Bay, Gulf of Mexico, TX contained pentachlorophenol at a range of 2.6-7.5 ppb; samples were collected from February to June, 1980(4). Pentachlorophenol has been detected in lake trout at concns of 357 pg/g wet weight (Lake Ontario), 504.2 pg/g wet weight (Lake Opeongo), and 244 pg/g wet weight (Lake Superior); sampling took place between May and August, 2000 and 2001(5).

Animal Concentrations:

Concentrations of this compound in animals.

>> After agricultural PCP application, birds can be highly contaminated (47 mg/kg wet weight in liver) ... PCP levels ranging from not detectable to 8571 ug/kg have been found in the muscle tissue of wild birds.

Average Daily Intake:

The average amount of the compound taken into the body through eating, drinking, or breathing.

>> The long-term, avg daily intake of pentachlorophenol is estimated to be 16 ug/day(1).

13. Disposal Considerations

Spillage Disposal

>> 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.

Disposal Methods

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste numbers D037; F027 must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> Pentachlorophenol is a waste chemical stream constituent which may be subjected to ultimate disposal by controlled incineration. Incineration (600 deg to 900 deg) coupled with adequate scrubbing and ash disposal facilities.

>> A potential candidate for rotary kiln incineration at a temperature range of 820 to 1,600 °C and residence times of seconds for liquids and gases, and hours for solids.

>> The following wastewater treatment technologies have been investigated for pentachlorophenol: Concentration process: Biological Treatment.

>> For more Disposal Methods (Complete) data for Pentachlorophenol (11 total), please visit the HSDB record page.

14. Transport Information

DOT

Pentachlorophenol
6.1
UN Pack Group: II
Reportable Quantity of 10 lb or 4

IATA

Pentachlorophenol
6.1,
UN Pack Group: II

15. Regulatory Information

Federal Drinking Water Standards:

Federal drinking water standards (e.g. maximum containment level (MCL)) for this chemical. These standards are legally enforceable.

>> Maximum contaminant levels (MCL) for synthetic organic contaminants apply to community water systems and non-transient, non-community water systems: Pentachlorophenol, MCL 0.001 mg/L.

Federal Drinking Water Guidelines:

Federal drinking water guidelines (e.g. maximum containment level (MCL)) for this chemical. In general, these guidelines are recommendations and not legally enforceable.

>> The maximum contaminant level goal for the following organic contaminant is zero mg/L: pentachlorophenol.

Clean Water Act Requirements:

The Clean Water Act (CWA) of 1972 establishes the basic structure for regulating discharges of pollutants into the waters of the United States and regulating quality standards for surface waters. Under CWA, the U.S. Environmental Protection Agency (EPA) developed the Toxic Pollutant List (40 CFR Part 401.15) and the Priority Pollutant List (40 CFR Part 423, Appendix A). These lists are to be used by EPA and States to develop the Effluent Guidelines regulations and ensure water quality criteria and standards.

>> Toxic pollutant designated pursuant to section 307(a)(1) of the Federal Water Pollution Control Act and is subject to effluent limitations.

Regulatory Information

REACH List of substances subject to POPs Regulation (POPs)

>> Substance: Pentachlorophenol

>> EC: 201-778-6

>> Date of inclusion in the POPs Regulation: 20-Jun-2019

>> POPs Regulation Annex: Annex I, part A

16. Other Information

Toxic Combustion Products:

Toxic products (e.g., gases and vapors) produced from the combustion of this chemical.

>> Poisonous gases including hydrogen chloride, dioxines, and chlorinated phenols are produced in fire.

Other Safety Information

Chemical Assessment

>> IMAP assessments - Phenol, pentachloro-: Environment tier I assessment

>> IMAP assessments - Phenol, pentachloro-: Human health tier I assessment

"The information provided is believed to be accurate but is not comprehensive and should be used as a reference. It reflects our current knowledge and is intended for safety guidance related to the product. This document does not constitute a warranty of the product's properties. Ionz is not responsible for any damages resulting from handling or contact with the product incorrectly."