

1. Material Identification

Product Name : 2-Chlorophenol

Catalog Number : io-1980

CAS Number : 95-57-8

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 (10.6%): Fatal if swallowed [Danger Acute toxicity, oral]

>> H302 (89.4%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H312 (100%): Harmful in contact with skin [Warning Acute toxicity, dermal]

>> H332 (100%): Harmful if inhaled [Warning Acute toxicity, inhalation]

>> H411 (100%): Toxic to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

Precautionary Statement Codes

>> P261, P264, P270, P271, P273, P280, P301+P316, P301+P317, P302+P352, P304+P340, P317, P321, P330, P362+P364, P391, P405, and P501

NFPA 704 Diamond



NFPA Health Rating

>> 2 – Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA Fire Rating

>> 2 – Materials that must be moderately heated or exposed to relatively high ambient temperatures before ignition can occur. Materials would not under normal conditions form hazardous atmospheres with air, but under high ambient temperatures or under moderate heating could release vapor in sufficient quantities to produce hazardous atmospheres with air.

NFPA Instability Rating

>> O – Materials that in themselves are normally stable, even under fire conditions.

Health Hazards:

- >> Poisonous; may be fatal if inhaled, swallowed or absorbed through skin. Irritating to skin and eyes; direct contact may cause burns. Rats receiving lethal doses via oral, subcutaneous or intraperitoneal routes displayed similar symptoms: restlessness, increased breathing rate and motor weakness followed by tremors, chronic convulsions, dyspnea, coma and death. (USCG, 1999)
- >> Special Hazards of Combustion Products: Contain poisonous chloride fumes.
- >> Behavior in Fire: Burns and produces toxic and irritating gases. (USCG, 1999)
- >> Combustible. Gives off irritating or toxic fumes (or gases) in a fire. Above 64 °C explosive vapour/air mixtures may be formed.

3. Composition/Information On Ingredients

Chemical name : 2-Chlorophenol
CAS Number : 95-57-8
Molecular Formula : C₆H₅ClO
Molecular Weight : 128.5500 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. If symptoms (such as wheezing, coughing, shortness of breath, or burning in the mouth, throat, or chest) develop, call a physician and be prepared to transport the victim to a hospital. 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. (NTP, 1992)

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 .

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. Do NOT induce vomiting. Refer for medical attention .

5. Fire Fighting Measures

- >> Fire Extinguishing Agents: Small fires: dry chemical, carbon dioxide, water spray or foam. Large Fires: Alcohol foam. (USCG, 1999)
- >> Excerpt from ERG Guide 153 [Substances – Toxic and/or Corrosive (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)
- >> Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

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 153 [Substances – Toxic and/or Corrosive (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)

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 vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in covered containers as far as possible. Carefully collect remainder. Then store and dispose of according to local regulations.

7. Handling And Storage

Safe Storage:

- >> Separated from strong oxidants and food and feedstuffs. Well closed.

Storage Conditions:

- >> Store in tightly closed containers in a cool, well ventilated area. Metal containers involving the transfer of this chemical should be grounded and bonded. Where possible, automatically pump liquid from drums or other storage containers to precess containers. Drums must be equipped with self-closing valves, pressure vacuum bungs, and flame arresters. Use only non-sparking tools and equipment, especially when opening and closing containers of this chemical. Sources of ignition such as smoking and open flames, are prohibited where this chemical is used, handled, or stored in a manner that could create a potential fire or explosion hazard. /Monochlorophenols/

8. Exposure Control/ Personal Protection

Inhalation Risk:

- >> No indication can be given about the rate at which a harmful concentration of this substance in the air is reached on evaporation at 20 °C.

Effects of Short Term Exposure:

- >> The substance is severely irritating to the eyes, skin and respiratory tract. Inhalation of the aerosol may cause lung oedema. The substance may cause effects on the central nervous system.

Fire Prevention

- >> NO open flames. Above 64 °C use a closed system and ventilation.

Exposure Prevention

- >> PREVENT GENERATION OF MISTS!

Inhalation Prevention

- >> Use ventilation, local exhaust or breathing protection.

Skin Prevention

- >> Protective gloves. Protective clothing.

Eye Prevention

- >> Wear face shield or eye protection in combination with breathing protection.

Ingestion Prevention

- >> Do not eat, drink, or smoke during work.

9. Physical And Chemical Properties

Molecular Weight:

- >> 128.55

Exact Mass:

- >> 128.0028925

Physical Description:

- >> 2-chlorophenol appears as a colorless to amber liquid with an unpleasant, penetrating odor. Density 1.265 g / cm³. Sinks in water and slowly dissolves. Freezing point 7 °C (46 °F). Boiling point 175 °C (347 °F).
- >> COLOURLESS LIQUID WITH CHARACTERISTIC ODOUR.

Color/Form:

- >> Light amber liquid

Odor:

- >> Unpleasant penetrating odor

Taste:

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

- >> Strong medicinal taste and odor

Boiling Point:

- >> 347 to 349 °F at 760 mmHg (NTP, 1992)
- >> 175 °C

Melting Point:

- >> 48.2 °F (NTP, 1992)
- >> 9.3–9.8 °C

Flash Point:

>> 147 °F (NTP, 1992)

>> 64 °C c.c.

Solubility:

>> 10 to 50 mg/mL at 59 °F (NTP, 1992)

>> Solubility in water, g/100ml at 20 °C: 2.85

Density:

>> 1.25 at 77 °F (USCG, 1999) – Denser than water; will sink

>> Relative density (water = 1): 1.3

Vapor Density:

>> Relative vapor density (air = 1): 4.4

Vapor Pressure:

>> 1 mmHg at 53.8 °F ; 2.2 mmHg at 68 °F (NTP, 1992)

>> Vapor pressure, Pa at 20 °C: 230

LogP:

>> log Kow = 2.15

>> 2.15

Decomposition:

>> When heated to decomposition it emits toxic fumes of /hydrogen chloride/.

Viscosity:

>> 3.579 cP at 25 °C

Heat of Combustion:

>> 2790.0 kJ.mol at 77 °F (liquid) /25 °C/

Heat of Vaporization:

>> 40.12 kJ/mole at 174.53 °C / 447.53 K/

pH:

pH is an expression of hydrogen ion concentration in water. Specifically, pH is the negative logarithm of hydrogen ion (H⁺) concentration (mol/L) in an aqueous solution. The term is used to indicate basicity or acidity of a solution on a scale of 0 to 14, with pH 7 being neutral.

>> weakly acidic

Surface Tension:

>> 40.50 dynes/cm at 25 °C

Odor Threshold:

>> Odor Threshold Low: 0.0036 [mmHg]

>> [ICSC] Odor threshold (threshold concentration) from CHEMINFO

Refractive Index:

>> Index of refraction: 1.5524 @ 20 °C

Dissociation Constants:

>> Ka = 3.2X10⁻⁹ at 25 °C

10. Stability And Reactivity

>> Very soluble in water

11. Toxicological Information

Toxicity Summary:

>> 2-chlorophenol works as a weak uncoupler of oxidative phosphorylation and inhibitors of cellular respiration. The ability of chlorophenols to uncouple oxidative phosphorylation increases with increasing chlorination. In fact, studies indicate a concentration-dependent triphasic effect of chlorophenols on phosphorylation and cellular respiration. At low concentrations, uncoupling produces stimulation of the resting state respiration as a result of increased adenosine triphosphatase (ATPase) activity in the absence of a phosphate acceptor. Inhibition of active respiration is also observed. At moderate concentrations, resting respiration is neither stimulated nor inhibited. Significant inhibition of respiration, associated with a breakdown of the electron transport process and decreased ATPase activity, occurs at very high concentrations. Uncoupling activity has been attributed to a protonophoric effect (a disruption of the energy gradient across the mitochondrial membrane resulting from distribution of chlorophenols in the phospholipid bilayer of the membrane), whereas inhibition of cellular respiration has been attributed to a direct action on intracellular proteins (L159).

EPA Provisional Peer-Reviewed Toxicity Values:

This section provides the EPA Provisional Peer-Reviewed Toxicity Values (PPRTVs) and links of related assessment documents.

Chemical Substance

>> 2-Chlorophenol

Reference Dose (RfD), Subchronic

>> 8×10^{-3} mg/kg-day

PPRTV Assessment

>> PDF Document

Weight-Of-Evidence (WOE)

>> Inadequate information to assess carcinogenic potential

Last Revision

>> 2007

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

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

Chemical

>> 2-Chlorophenol

Noncancer HBSL (Health-Based Screening Level)[$\mu\text{g/L}$]

>> 30

Reference

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

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).

>> No indication of carcinogenicity (not listed by IARC). (L135)

Health Effects:

>> 2-chlorophenol is corrosive to epithelial tissue. It produce effects ranging from slight hyperemia to severe corrosion when applied to the corneas. Acute inhalation exposure may lead to hemorrhage in the lungs and tachypnea. Oral exposure to 2-chlorophenol can produce a variety of neurological effects, including tremors, myoclonic convulsions, a hunched posture, dyspnea, collapse, and coma (L159).

Exposure Routes:

>> The substance can be absorbed into the body by inhalation of its vapour, through the skin and by ingestion.
>> Inhalation (L723) ; oral (L723) ; dermal (L723)

Inhalation Exposure

>> Cough. Shortness of breath. Sore throat. See Ingestion. Symptoms may be delayed.

Skin Exposure

>> MAY BE ABSORBED! Redness. Pain.

Eye Exposure

>> Redness. Pain. Blurred vision.

Ingestion Exposure

>> Abdominal pain. Drowsiness. Weakness. Convulsions.

>> Cough, shortness of breath and sore throat can result from inhalation of 2-chlorophenol. These symptoms may be delayed. Abdominal pain, drowsiness, weakness, and convulsions can result from ingestion as well as inhalation. Moreover, ingestion of 2-chlorophenol can cause restlessness, tremors, or central nervous system depression to occur. Eye exposure to 2-chlorophenol can lead to redness, pain, and blurred vision, while dermal contact can lead to redness and pain of the skin. Moreover, the substance can be rapidly absorbed after derma exposure (L723).

Target Organs:

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

>> Reproductive

Adverse Effects:

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

>> Neurotoxin – Other CNS neurotoxin

>> 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.

>> Dermatotoxin – Skin burns.

Toxicity Data:

>> LC50 (rat) = 390 ppm/4hr

Treatment:

Treatment when exposed to toxin

>> Avoid dilution following oral exposure; instead, administer charcoal as a slurry. Following inhalation, move patient to fresh air. Monitor for respiratory distress. If cough or difficulty breathing develops, evaluate for respiratory tract irritation, bronchitis, or pneumonitis. Administer oxygen and assist ventilation as required. Treat bronchospasm with inhaled beta2 agonist and oral or parenteral corticosteroids. In case the exposure occurs through eye contact, irrigate exposed eyes with copious amounts of room temperature water for at least 15 minutes. Following dermal exposure, remove phenol with undiluted polyethylene glycol 300 to 400 or isopropyl alcohol prior to washing, if readily available. Wash exposed areas twice or for at least 10 minutes with large quantities of soapy water. Water alone may be harmful. (T36)

Interactions:

>> Tumor incidence incr (69%) in rats receiving 2-chlorophenol (5 ppm) and ethylnitrosourea, as compared to 58% for rats receiving ethylnitrosourea only. The effects of 2-chlorophenol on reproduction might be related to the transplacental transfer of 2-chlorophenol.

Antidote and Emergency Treatment:

>> Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. /Phenols and related compounds/

Human Toxicity Excerpts:

>> /SIGNS AND SYMPTOMS/ Caution: ingestion causes incr then decr of respiration, blood pressure, urinary output; fever; increased bowel action; motor weakness; collapse with convulsions & death. Causes lung, liver, kidney damage, contact dermatitis. ... Dust causes sneezing.

Non-Human Toxicity Excerpts:

>> /LABORATORY ANIMALS: Acute Exposure/ In rats oral, subcutaneous, and intraperitoneal lethal doses of the chlorophenols produce similar signs of poisoning. Oral administration, however, results in fatal poisoning in smaller

dosage and in a shorter period of time than sc administration. /Chlorophenols/

Non-Human Toxicity Values:

>> LD50 Rat oral 670 mg/kg. /From table/

12. Ecological Information

Resident Soil (mg/kg)

>> 3.90e+02

Industrial Soil (mg/kg)

>> 5.80e+03

Tapwater (ug/L)

>> 9.10e+01

MCL (ug/L)

>> 8.0E+01(G)

Risk-based SSL (mg/kg)

>> 8.90e-02

Chronic Oral Reference Dose (mg/kg-day)

>> 5.00e-03

Volatile

>> Volatile

Mutagen

>> Mutagen

Fraction of Contaminant Absorbed in Gastrointestinal Tract

>> 1

Soil Saturation Concentration (mg/kg)

>> 2.74e+04

ICSC Environmental Data:

>> The substance is toxic to aquatic organisms. The substance may cause long-term effects in the aquatic environment.

Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SOIL: 2-Chlorophenol was identified in soil samples taken from the Ville Mercier site (12 different locations) in southern Quebec, Canada, in concns ranging from 1.1 to 12,350 ug/kg(1). The concn of 2-chlorophenol in river sediments above and below the effluent discharges of two New Zealand pulp and paper mills was determined to range from 0 to 0.5 ng/g(2). Samples were collected from a remedial investigation site located north of Lake Pontchartrain in Slidell, LA in February 1986; the concn of 2-chlorophenol in sediment from the Bayou Bonfouca site was determined to be 3,000 ug/kg (ppb)(3). USEPA STORET database: 308 samples, 1% pos, median, <1,000 ppm(4).

Fish/Seafood Concentrations:

Concentrations of this compound in fish or seafood.

>> -Chlorophenol was identified, but not quantified, in various fish collected from Lake Michigan and tributary streams during 1983(1). 2-Chlorophenol was detected in composite fish samples collected from the Great Lakes Harbors and Tributaries between 1980 and 1981, concn unknown(2).

13. Disposal Considerations

Spillage Disposal

- >> Personal protection: chemical protection suit and filter respirator for organic gases and vapours adapted to the airborne concentration of the substance. Do NOT let this chemical enter the environment. Collect leaking and spilled liquid in covered containers as far as possible. 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 number U048, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.
- >> Good candidate for rotary kiln incineration, with a temperature range of 820 to 1600 °C and a residence time of seconds. Also, a good candidate for liquid injection incineration, with a temperature range of 650 to 1600 °C and a residence time of 0.1 to 2 seconds.
- >> This paper reports a three-step approach to remove 2-chlorophenol from dilute aqueous solution and compares each technique. The first step utilizes Horse Radish Peroxidase (HRP) in presence of hydrogen peroxide to oxidize this organic pollutant (enzyme treatment). For a more efficient removal of 2-chlorophenol, it is necessary to add the enzyme solution gradually to the contents of the reactor instead of rapid addition. The second step, involving ultrasonic waves eliminated 2-chlorophenol through hydroxyl radical generated by the cavitation process (sono-degradation). In the third step, a combination of ultrasonic waves and enzyme was used (sono-enzyme degradation).
- >> Wet oxidation of a 100 ppm aqueous solution of o-chlorophenol (o-CP) was performed in a lab-scale batch reactor using 3% Ru/TiO₂ catalyst at 373 and 413 K, and a partial oxygen pressure of 0.1 MPa. The experiments were conducted by varying the initial pH values of o-CP solution from pH 6.3 to 9.8 and 11.8. From the results, it was revealed that the catalytic decomposition of o-CP occurred most effectively at 413 K and at the initial pH of 9.8. Complete decomposition and dechlorination of o-CP were almost achieved within 1hr, and about 85% of TOC was removed in 3.0 hr...
- >> For more Disposal Methods (Complete) data for 2-CHLOROPHENOL (14 total), please visit the HSDB record page.

14. Transport Information

DOT

2-Chlorophenol

6.1

UN Pack Group: III

Reportable Quantity of 100 lb or 45

IATA

2-Chlorophenol

6.1,

UN Pack Group: III

15. Regulatory Information

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.

- >> EPA 40 ug/L

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

The Australian Inventory of Industrial Chemicals

>> Chemical: Phenol, 2-chloro-

The Australian Inventory of Industrial Chemicals

>> Chemical: Phenol, chloro-

REACH Registered Substance

>> Status: Active Update: 01-03-2017 <https://echa.europa.eu/registration-dossier/-/registered-dossier/19031>

>> Status: Active Update: 26-04-2013 <https://echa.europa.eu/registration-dossier/-/registered-dossier/6091>

>> Status: Active Update: 27-09-2018 <https://echa.europa.eu/registration-dossier/-/registered-dossier/21842>

New Zealand EPA Inventory of Chemical Status

>> 2-Chlorophenol: Does not have an individual approval but may be used under an appropriate group standard

16. Other Information

Toxic Combustion Products:

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

>> Poisonous gases including phenols and chlorides are produced in fire.

Other Safety Information

Chemical Assessment

>> Evaluation – Chemicals not considered for in depth evaluation – Not commercially active in Australia

"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."