# SAFETY DATA SHEET

Updated on 26/09/2024

## 1. Material Identification

**Product Name** : p-Chloro-m-cresol
**Catalog Number** : io-1964
**CAS Number** : 59-50-7
**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**

>> H302 (100%): Harmful if swallowed [Warning Acute toxicity, oral]

>> H312 (92.2%): Harmful in contact with skin [Warning Acute toxicity, dermal]

>> H314 (19.9%): Causes severe skin burns and eye damage [Danger Skin corrosion/irritation]

>> H317 (99.9%): May cause an allergic skin reaction [Warning Sensitization, Skin]

>> H318 (100%): Causes serious eye damage [Danger Serious eye damage/eye irritation]

>> H335 (19%): May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation]

>> H400 (99.9%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

>> H412 (19%): Harmful to aquatic life with long lasting effects [Hazardous to the aquatic environment, long-term hazard]

**Precautionary Statement Codes**

>> P260, P261, P264, P264+P265, P270, P271, P272, P273, P280, P301+P317, P301+P330+P331, P302+P352, P302+P361+P354, P304+P340, P305+P354+P338, P316, P317, P319, P321, P330, P333+P317, P362+P364, P363, P391, P403+P233, P405, and P501

### Health Hazards:

>> Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]:

>> Highly toxic, may be fatal if inhaled, ingested or absorbed through skin. 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. (ERG, 2024)

>> Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]:

>> Combustible material: may burn but does not ignite readily. Containers may explode when heated. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2024)

>> Combustible. Gives off irritating or toxic fumes (or gases) in a fire.

## 3. Composition/Information On Ingredients

**Chemical name** : p-Chloro-m-cresol
**CAS Number** : 59-50-7
**Molecular Formula** : C7H7ClO
**Molecular Weight** : 142.5800 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. Refer for medical attention.

#### Skin First Aid

>> Remove contaminated clothes. Rinse skin with plenty of water or shower. 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. Refer for medical attention .

## 5. Fire Fighting Measures

>> Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]:

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

>> LARGE FIRE: Water spray, fog or regular foam. If it can be done safely, move undamaged containers away from the area around the fire. Dike runoff from fire control for later disposal. Avoid aiming straight or solid streams directly onto the product.

>> 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. For massive fire, use unmanned master stream devices or monitor nozzles; if this is impossible, withdraw from area and let fire burn. (ERG, 2024)

>> Use water spray, powder.

## 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 152 [Substances - Toxic (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 including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

## 7. Handling And Storage

### Safe Storage:

>> Separated from food and feedstuffs. Dry.

## 8. Exposure Control/ Personal Protection

### Inhalation Risk:

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

### Effects of Short Term Exposure:

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

### Effects of Long Term Exposure:

>> Repeated or prolonged contact may cause skin sensitization.

**Fire Prevention**

>> NO open flames.

**Exposure Prevention**

>> PREVENT DISPERSION OF DUST! AVOID ALL CONTACT!

**Inhalation Prevention**

>> Use local exhaust or breathing protection.

**Skin Prevention**

>> Protective gloves.

**Eye Prevention**

>> Wear safety goggles 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:**

>> 142.58

**Exact Mass:**

>> 142.0185425

**Physical Description:**

>> Chlorocresol appears as a pinkish to white crystalline solid with a phenolic odor. Melting point 64-66 °C. Shipped as a solid or in a liquid carrier. Soluble in aqueous base. Toxic by ingestion, inhalation or skin absorption. Used as an external germicide. Used as a preservative in paints and inks.

>> WHITE OR SLIGHTLY PINK HYGROSCOPIC CRYSTALS OR CRYSTALLINE POWDER.

**Color/Form:**

>> Dimorphous crystals ... aqueous solutions turn yellow on exposure to light and air

**Odor:**

>> Said to be odorless when very pure, but usually a phenolic odor persists

**Boiling Point:**

>> 455 °F at 760 mmHg (NTP, 1992)

>> 235 °C

**Melting Point:**

>> 151 °F (NTP, 1992)

>> 66 °C

**Flash Point:**

>> 230 °F (NTP, 1992)

>> 118 °C

**Solubility:**

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

>> Solubility in water, g/100ml at 20 °C: 0.38

**Density:**

>> 0.9 at 77 °F (NTP, 1992) - Less dense than water; will float

>> 1.4 g/cm$^3$

**Vapor Pressure:**

>> 0.05 [mmHg]

**LogP:**

>> log Kow = 3.10

>> 3.1

**Stability/Shelf Life:**

>> Aq solns turn yellow on exposure to light and air.

**Autoignition Temperature:**

>> 590 °C

**Decomposition:**

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

**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.

>> pH = 5.6 in saturated aqueous solution

**Odor Threshold:**

>> detection: 0.1 mg/kg

**Dissociation Constants:**

>> pKa = 9.55

**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.

>> 123.36 Å² [M+H]+ [CCS Type: TW; Method: calibrated with polyalanine and drug standards]

## 10. Stability And Reactivity

>> Hygroscopic. Soluble in aqueous base.

## 11. Toxicological Information

**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**

>> p-Chloro-m-cresol

**PPRTV Assessment**

>> PDF Document

**Weight-Of-Evidence (WOE)**

>> Inadequate information to assess carcinogenic potential

**Last Revision**

>> 2018

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

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

**Chemical**

>> p-Chloro-m-cresol

**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).

>> Cancer Classification: Group D Not Classifiable as to Human Carcinogenicity

**Exposure Routes:**

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

**Inhalation Exposure**

>> Cough. Sore throat. See Ingestion.

**Skin Exposure**

>> Redness. Pain.

**Eye Exposure**

>> Redness. Pain. Severe deep burns.

**Ingestion Exposure**

>> Headache. Dizziness. Shortness of breath. Abdominal pain. Vomiting. Diarrhoea.

**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.

>> Methemoglobinemia - The presence of increased methemoglobin in the blood; the compound is classified as secondary toxic effect

>> Dermatotoxin - Skin burns.

>> Skin Sensitizer - An agent that can induce an allergic reaction in the skin.

**Interactions:**

>> The toxicity of phenol to filamentous fungi was unaffected by pH or water hardness... . ...An antagonistic interaction in toxicity occurred between phenol and ...p-chloro-m-cresol.

**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:**

>> /HUMAN EXPOSURE STUDIES/ No skin reaction was observed in volunteers after intradermal injections of 0.3 mL 3-methyl-4-chlorophenol solution (= 1.5 mg) in the forearm (observation time: 4 hr). 3-methyl-4-chlorophenol solution (2 %) was incorporated in a lot of dressing and placed on the sacrificed arm of a volunteer of one week; dermal reactions were not observed.

**Non-Human Toxicity Excerpts:**

>> /LABORATORY ANIMALS: Acute Exposure/ Groups of male Wistar rats were given a single oral dose of 400 mg/kg PCMC in peanut oil; controls were dosed with an equivalent amount of peanut oil only. All animals were killed 60 hr after dosing, and hepatic tissue was removed from the center of the right lobe of the liver for examination by electron microscopy. After dosing, the animals' behavior changed; after 30 minutes, the animals were uneasy and had "ruffled-up" coats. These signs diminished after 1 hr, but they were replaced by long "apathetic motions". After 24 hr until study termination, the hair coats were again altered. At necropsy, the liver appeared slightly enlarged and was a pale red color with pale gray spots. Light microscopy findings included a distinct dilation of the sinusoids with an activation of the Kupffer cells. The intercellular spaces were enlarged, and there were numerous vacuoles found in the cytoplasm. In electron micrographs, outpouchings of cell membranes were observed. A greater than normal number of lysosomes were around the bile canaliculi after dosing. Also, there was an increase in the number of mitochondria, many membrane-surrounded vacuoles, alterations in the intercellular space and in the rough endoplasmic reticulum, and an increase in the number and size of gap junctions. Additionally, the bile canaliculi were dilated and had irregularities and side branches which extended into the cytoplasm of adjacent hepatocytes.

**Non-Human Toxicity Values:**

>> LD50 Rat dermal > 2000 mg/kg bw

**Populations at Special Risk:**

>> /4-Chloro-m-cresol/ is a preservative within a large number of commercially available preparations (e.g. insulin, hormones, etc.). Regarding the results of contracture testing with 4-CmC it has been suggested that 4-CmC possibly represents a high-risk agent for /malignant hyperthermia susceptible/ individuals. To reduce the risk of /malignant hyperthermia/ in susceptible patients due to administration of chlorocresols, .../avoid/ preparations containing the preservative 4-CmC.

## 12. Ecological Information

**Resident Soil (mg/kg)**

>> 6.30e+03

**Industrial Soil (mg/kg)**

>> 8.20e+04

**Tapwater (ug/L)**

>> 1.40e+03

**MCL (ug/L)**

>> 1.30e+03

**Risk-based SSL (mg/kg)**

>> 1.70e+00

**Chronic Oral Reference Dose (mg/kg-day)**

>> 1.00e-01

**Volatile**

>> Volatile

**Mutagen**

>> Mutagen

**Fraction of Contaminant Absorbed in Gastrointestinal Tract**

>> 1

**Fraction of Contaminant Absorbed Dermally from Soil**

>> 0.1

### ICSC Environmental Data:

>> The substance is toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish.

### Sediment/Soil Concentrations:

Concentrations of this compound in sediment/soil.

>> SEDIMENT: 3-Methyl-4-chlorophenol has been qualitatively detected in the soil-sediment matrix of the Love Canal waste disposal site near Niagara Falls, NY(1). 3-Methyl-4-chlorophenol had a frequency of detection of 0.2% in streambed sediment samples taken at 489 sites from 20 major river basins across the United States from 1992 to 1995(2). The concentration at the 95th percentile was less than 50 ug/kg with a maximum concentration of 190 ug/kg(2). 3-Methyl-4-chlorophenol was detected with a maximum concentration of 3000 ug/kg in soil and sediment at the Bayou Bonfouca hazardous waste site in Slidell, Louisiana(3). This site is listed on the National Priorities list of Superfund sites(3).

## 13. Disposal Considerations

**Spillage Disposal**

>> Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered sealable containers. If appropriate, moisten first to prevent dusting. Then store and dispose of according to local regulations.

### Disposal Methods

>> SRP: The most favorable course of action is to use an alternative chemical product with less inherent propensity for occupational harm/injury/toxicity or environmental contamination. Recycle any unused portion of the material for its approved use or return it to the manufacturer or supplier. Ultimate disposal of the chemical must consider: the material's impact on air quality; potential migration in soil or water; effects on animal and plant life; and conformance with environmental and public health regulations.

>> Generators of waste (equal to or greater than 100 kg/mo) containing this contaminant, EPA hazardous waste number U039, must conform with USEPA regulations in storage, transportation, treatment and disposal of waste.

>> A good 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.

>> A pilot plant study was conducted to evaluate the fate and behavior of 22 toxic organic compounds in conventional activated sludge wastewater treatment plants. The organic cmpd, 3-methyl-4-chlorophenol, spiked at a nominal concn of 50 ug/L was about 95-98% removable. Results showed that biodegradability was variable & was a function of molecular structure.

## 14. Transport Information

### DOT

p-Chloro-m-cresol
6.1
UN Pack Group: II
Reportable Quantity of 5000 lb or 2270 kg

### IATA

p-Chloro-m-cresol
6.1,
UN Pack Group: II

## 15. Regulatory Information

### 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. Chlorinated phenols (includes trichlorophenols and chlorinated cresols)/

### Regulatory Information

#### The Australian Inventory of Industrial Chemicals

>> Chemical: Phenol, 4-chloro-3-methyl-

#### REACH Registered Substance

>> Status: Active Update: 29-09-2021 https://echa.europa.eu/registration-dossier/-/registered-dossier/10359

#### New Zealand EPA Inventory of Chemical Status

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

## 16. Other Information

### Other Safety Information

### Chemical Assessment

>> IMAP assessments - Chlorocresol and its sodium salt: Human health tier II assessment

>> Evaluation - Chlorocresol and chloroxylenol

"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."