

Chemical Safety Data Sheet MSDS / SDS

4-Chloro-3-methylphenol

Revision Date:2023-12-07 Revision Number:1

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

Product identifier

Product name : 4-Chloro-3-methylphenol
CBnumber : CB5703115
CAS : 59-50-7
EINECS Number : 200-431-6
Synonyms : Chlorocresol,PCMC

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
Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing
Telephone : 400-158-6606

SECTION 2: Hazards identification

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to.....

P405 Store locked up.

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

P391 Collect spillage. Hazardous to the aquatic environment

P314 Get medical advice/attention if you feel unwell.

P311 Call a POISON CENTER or doctor/physician.

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

Continuerinsing.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

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

P273 Avoid release to the environment.
P272 Contaminated work clothing should not be allowed out of the workplace.
P271 Use only outdoors or in a well-ventilated area.
P270 Do not eat, drink or smoke when using this product.
P264 Wash skin thoroughly after handling.
P264 Wash hands thoroughly after handling.
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

Hazard statements

H410 Very toxic to aquatic life with long lasting effects
H400 Very toxic to aquatic life
H373 May cause damage to organs through prolonged or repeated exposure
H370 Causes damage to organs
H335 May cause respiratory irritation
H318 Causes serious eye damage
H317 May cause an allergic skin reaction
H312 Harmful in contact with skin
H302 Harmful if swallowed
H225 Highly Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: 4-Chloro-3-methylphenol
Synonyms	: Chlorocresol,PCMC
CAS	: 59-50-7
EC number	: 200-431-6
MF	: C7H7ClO
MW	: 142.58

SECTION 4: First aid measures

Description of first aid measures

General advice

First aiders need to protect themselves. Show this material safety data sheet to the doctor

If inhaled

After inhalation: fresh air. Call in physician.

In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Call a physician immediately.

In case of eye contact

After eye contact: rinse out with plenty of water. Immediately call in ophthalmologist. Remove contact lenses.

If swallowed

After swallowing: make victim drink water (two glasses at most), avoid vomiting (risk of perforation). Call a physician immediately. Do not attempt to neutralise.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media

Suitable extinguishing media

Water Foam Carbon dioxide (CO₂) Dry powder

Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

Special hazards arising from the substance or mixture

Carbon oxides Hydrogen chloride gas Combustible.

Vapors are heavier than air and may spread along floors. Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

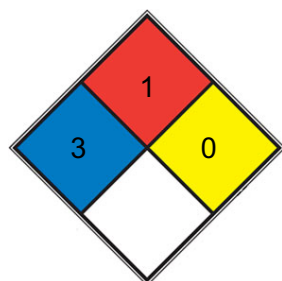
Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

Further information

Suppress (knock down) gases/vapors/mists with a water spray jet. Prevent fire extinguishing water from contaminating surface water or the ground water system.

NFPA 704



■ HEALTH 3 Short exposure could cause serious temporary or moderate residual injury (e.g. [liquid hydrogen](#), [sulfuric acid](#), [calcium hypochlorite](#), hexafluorosilicic acid)

■ FIRE 1 Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. [mineral oil](#), ammonia)

REACT 0 Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N2](#))

SPEC.

HAZ.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert.

For personal protection see section 8.

Environmental precautions

Do not let product enter drains.

Methods and materials for containment and cleaning up

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Advice on safe handling

Work under hood. Do not inhale substance/mixture.

Hygiene measures

Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Storage conditions

Tightly closed. Dry. Keep in a well-ventilated place. Keep locked up or in an area accessible only to qualified or authorized persons.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Personal protective equipment

Eye/face protection

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Tightly fitting safety goggles

Skin protection

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatril? L

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN374 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: www.kcl.de).

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,11 mm Break through time: 480 min

Material tested:KCL 741 Dermatril? L

Body Protection

protective clothing

Respiratory protection

Recommended Filter type: Filter A-(P2)

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer.

These measures have to be properly documented.

Control of environmental exposure

Do not let product enter drains.

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	colorless solid
Odour	characteristic
Odour Threshold	No data available
pH	5,25 at 30 °C
Melting point/freezing point	Melting point/range: 63 - 65 °C - lit.
Initial boiling point and boiling range	235 °C - lit.

Flash point	118,0 °C - closed cup - DIN 51758
Evaporation rate	No data available
Flammability (solid, gas)	The product is not flammable.
Upper/lower flammability or explosive limits	No data available
Vapour pressure	6,9 hPa at 100,0 °C 0,1 hPa at 20,0 °C
Vapour density	No data available
Relative density	No data available
Water solubility	4 g/l at 30 °C - soluble
Partition coefficient: n-octanol/water	log Pow: 0,47 at 30 °C - Bioaccumulation is not expected.
Autoignition temperature	590,0 °C
Decomposition temperature	200,0 °C -
Viscosity	Viscosity, kinematic: No data available Viscosity, dynamic: No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	$2.5 \times 10^{-6} \text{ atm} \cdot \text{m}^3/\text{mol}$ at 20 °C (calculated, Mabey et al., 1982)

Other safety information

Surface tension 61,49 mN/m at 1g/l at 20 °C

Surface tension

Dissociation constant 9,4 at 20 °C

OECD Test Guideline 112

SECTION 10: Stability and reactivity

Reactivity

Forms explosive mixtures with air on intense heating.

A range from approx. 15 Kelvin below the flash point is to be rated as critical.

The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.

Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

Possibility of hazardous reactions

Violent reactions possible with:

Oxidizing agents Acid anhydrides acid halides Bases

Conditions to avoid

Strong heating.

Incompatible materials

Copper, Copper alloys, brass, Mild steel

Hazardous decomposition products

In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male - 1.830 mg/kg

(OECD Test Guideline 401)

LC50 Inhalation - Rat - male and female - 4 h - > 2,87 mg/l (OECD Test Guideline 403)

Symptoms: Possible damages:, Lung edema, mucosal irritations LD50 Dermal - Rat - female - 2.000 mg/kg

(OECD Test Guideline 402)

Skin corrosion/irritation

Skin - Rabbit

Result: Corrosive after 1 to 4 hours of exposure (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes burns. - 24 h (OECD Test Guideline 405) Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)

Respiratory or skin sensitization

Maximization Test - Guinea pig

Result: positive

(OECD Test Guideline 406)

Germ cell mutagenicity

UDS (Unscheduled DNA synthesis assay) rat hepatocytes

Result: negative Ames test

S. typhimurium Result: negative

In vitro mammalian cell gene mutation test Chinese hamster ovary cells

Result: negative

OECD Test Guideline 474

Mouse - male and female - Bone marrow Result: negative

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

No data available

Specific target organ toxicity - single exposure

May cause respiratory irritation. Remarks:

Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2) Acute inhalation toxicity - Possible damages:, Lung edema, mucosal irritations

Specific target organ toxicity - repeated exposure

No data available

Aspiration hazard

No data available

Toxicity

LD50 orally in Rabbit: 1830 mg/kg LD50 dermal Rat > 2000 mg/kg

SECTION 12: Ecological information

Toxicity

Toxicity to fish

semi-static test LC50 - *Oncorhynchus mykiss* (rainbow trout) - 0,917

Toxicity to daphnia and other aquatic invertebrates

mg/l - 96 h (US-EPA)

static test EC50 - *Daphnia magna* (Water flea) - 2,29 mg/l - 48 h (US-EPA)

Toxicity to algae

static test ErC50 - *Desmodesmus subspicatus* (green algae) - 30,62 mg/l - 72 h
(OECD Test Guideline 201)

static test NOEC - *Desmodesmus subspicatus* (green algae) - 9,8 mg/l - 72 h
(OECD Test Guideline 201)

Toxicity to bacteria

static test EC50 - activated sludge - 41,4 mg/l - 3 h
(OECD Test Guideline 209)

Persistence and degradability

Biodegradability aerobic - Exposure time 28 d

Result: 85 % - Readily biodegradable. (OECD Test Guideline 301D)

Theoretical oxygen demand

1.852 mg/g

Bioaccumulative potential

Bioaccumulation *Cyprinus carpio* (Carp) - 6 Weeks

at 25 °C - 0,002 mg/l(chlorocresol)

Bioconcentration factor (BCF): 5,5 - 11

Mobility in soil

No data available

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

Discharge into the environment must be avoided.

SECTION 13: Disposal considerations

Waste treatment methods

Incompatibilities

Chlorocresol can decompose on contact with strong alkalis, evolving heat and fumes that ignite explosively. It is also incompatible with oxidizing agents, copper, and with solutions of calcium chloride, codeine phosphate, diamorphine hydrochloride, papaveretum, and quinine hydrochloride.

Product

See www.retrologistik.com for processes regarding the return of chemicals and containers, or contact us there if you have further questions.

Waste Disposal

A good candidate for rotary kiln incineration at a temperature range of 820 to 1600C and residence times of seconds for liquids and gases, and hours for solids.

SECTION 14: Transport information

UN number

ADR/RID: 3437 IMDG: 3437 IATA: 3437

UN proper shipping name

ADR/RID: CHLOROCRESOLS, SOLID (chlorocresol)

IMDG: CHLOROCRESOLS, SOLID (chlorocresol) IATA: Chlorocresols, solid (chlorocresol)

Transport hazard class(es)

ADR/RID: 6.1 IMDG: 6.1 IATA: 6.1

Packaging group

ADR/RID: II IMDG: II IATA: II

Environmental hazards

ADR/RID: yes IMDG Marine pollutant: yes IATA: no

Special precautions for user

No data available

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015:Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Listed. website: <https://www.mee.gov.cn/>

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory:Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC):Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL):Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS):Listed. website: <https://echa.europa.eu/>

EC Inventory:Listed.

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

[1] CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

[2] ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

[3] ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

[4] eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

[5] ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

[6] Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

[7] HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

[8] IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

[9] IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

[10] Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

Disclaimer:

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