

Chemical Safety Data Sheet MSDS / SDS

2-methyl-4,6-dinitro-phenol SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: 2-methyl-4,6-dinitro-phenol

CAS: 534-52-1

Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.

Uses advised against: none

Company Identification

Company: Chemicalbook.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Acute toxicity - Category 2, Oral

Acute toxicity - Category 1, Dermal

Skin irritation, Category 2
Serious eye damage, Category 1
Skin sensitization, Category 1
Acute toxicity - Category 2, Inhalation
Germ cell mutagenicity, Category 2
Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1
Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Danger

Hazard statement(s)

H300 Fatal if swallowed
H310 Fatal in contact with skin
H315 Causes skin irritation
H318 Causes serious eye damage
H317 May cause an allergic skin reaction
H330 Fatal if inhaled
H341 Suspected of causing genetic defects
H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

P264 Wash ... thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P262 Do not get in eyes, on skin, or on clothing.
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.
P272 Contaminated work clothing should not be allowed out of the workplace.
P260 Do not breathe dust/fume/gas/mist/vapours/spray.
P271 Use only outdoors or in a well-ventilated area.
P284 [In case of inadequate ventilation] wear respiratory protection.
P203 Obtain, read and follow all safety instructions before use.
P273 Avoid release to the environment.

Response

P301+P316 IF SWALLOWED: Get emergency medical help immediately.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

P302+P352 IF ON SKIN: Wash with plenty of water/...

P316 Get emergency medical help immediately.

P361+P364 Take off immediately all contaminated clothing and wash it before reuse.

P332+P317 If skin irritation occurs: Get medical help.

P362+P364 Take off contaminated clothing and wash it before reuse.

P305+P354+P338 IF IN EYES: Immediately rinse with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.

P317 Get medical help.

P333+P317 If skin irritation or rash occurs: Get medical help.

P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P320 Specific treatment is urgent (see ... on this label).

P318 IF exposed or concerned, get medical advice.

P391 Collect spillage.

Storage

P405 Store locked up.

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

Disposal

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

Other hazards which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name: 2-methyl-4,6-dinitro-phenol

Common names and synonyms: 2-methyl-4,6-dinitro-phenol

CAS number: 534-52-1
EC number: 208-601-1
Concentration: 100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Artificial respiration may be needed. Refer for medical attention.

Following skin contact

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

Following eye contact

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

Following ingestion

Rinse mouth. Give a slurry of activated charcoal in water to drink. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Extremely toxic material; probable oral lethal dose is 5-50 mg/kg in humans or between 7 drops and 1 teaspoonful for a 70 kg (150 lb.) person. (EPA, 1998)

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

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. Dinitrophenol and Related Compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Extinguish fire using agent suitable for type of surrounding fire. (Material itself does not burn or burns with difficulty.) Keep run-off water out of sewers and water sources.

Specific hazards arising from the chemical

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: Combustible material: may burn but does not ignite readily. When heated, vapors may form explosive mixtures with air: indoors, outdoors and sewers explosion hazards. Those substances designated with a (P) may polymerize explosively when heated or involved in a fire. Contact with metals may evolve flammable hydrogen gas. Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)

Special protective actions for fire-fighters

Use water spray, foam, dry powder, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

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. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

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. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Environmental considerations: Land spill: Dig a pit, pond lagoon, holding area to contain liquid or solid material. /SRP: If time permits, pits, ponds, lagoons, soak holes, or holding areas should be sealed with an impermeable flexible membrane liner./ Cover solids with a plastic sheet to prevent dissolving in rain or fire fighting water.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. NO contact with oxidizing agents. Closed system, dust explosion-proof electrical equipment and lighting. Prevent deposition of dust. Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

Conditions for safe storage, including any incompatibilities

Separated from strong oxidants and food and feedstuffs. Well closed. You should protect this material from exposure to light, and store it in a refrigerator.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.2 mg/m³, as TWA; (skin). MAK: skin absorption (H)

Biological limit values

no data available

Appropriate engineering controls

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

Individual protection measures, such as personal protective equipment (PPE)

Eye/face protection

Wear safety goggles or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	4,6-dinitro-o-cresol is a yellow solid. Emits toxic oxides of nitrogen fumes when heated to decomposition. Toxic by skin absorption, inhalation or ingestion. Soluble in alcohol, acetone, ether and solutions of sodium or potassium hydroxides.
Colour:	Yellow prisms from alcohol
Odour:	Odorless
Melting point/freezing point:	83-85°C
Boiling point or initial boiling point and boiling range:	332.4°C at 760 mmHg
Flammability:	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	149.2°C
Auto-ignition temperature:	340°C
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	0.01 % (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow = 2.13
Vapour pressure:	5e-05 mm Hg (EPA, 1998)

Density and/or relative density:	1.55 g/cm ³
Relative vapour density:	6.82 (EPA, 1998) (Relative to Air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic fumes including nitrogen oxides. Reacts violently with strong oxidants.

Chemical stability

Stable during transport.

Possibility of hazardous reactions

Dust explosion possible if in powder or granular form, mixed with air. This compound is incompatible with the following: Strong oxidizers (NIOSH, 2016). Phenols do not behave as organic alcohols, as one might guess from the presence of a hydroxyl (-OH) group in their structure. Instead, they react as weak organic acids. Phenols and cresols are much weaker as acids than common carboxylic acids (phenol has pKa = 9.88). These materials are incompatible with strong reducing substances such as hydrides, nitrides, alkali metals, and sulfides. Flammable gas (H₂) is often generated, and the heat of the reaction may ignite the gas. Heat is also generated by the acid-base reaction between phenols and bases. 4,6-DINITRO-O-CRESOL is explosive and is usually moistened with up to 10 percent water to reduce the hazard. [EPA, 1998].

Conditions to avoid

no data available

Incompatible materials

Strong oxidizers.

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of /nitrogen oxides/.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Rat oral 10 mg/kg.

Inhalation: no data available

Dermal: LD50 Rabbit percutaneous 1,000 mg/kg

Skin corrosion/irritation

no data available

Serious eye damage/irritation

no data available

Respiratory or skin sensitization

no data available

Germ cell mutagenicity

no data available

Carcinogenicity

no data available

Reproductive toxicity

no data available

STOT-single exposure

The substance is corrosive to the eyes. The substance is irritating to the skin. The substance may cause effects on the metabolic rate. Exposure at high levels could cause death.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will not or will only very slowly be reached on evaporation of this substance at 20°C; on spraying or dispersing, however, much faster.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: Danio rerio (Zebra danio) length 2.5 cm; Conditions: freshwater, static, 22 deg C, pH 7.8-8, hardness 150 mg/L CaCO₃; Concentration: 1000-3500 ug/L for 24 hr

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater, renewal, 25 deg C, pH >7; Concentration: 2300 ug/L for 24 hr; Effect: behavior, equilibrium /formulation

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: In a static-culture flask-screening procedure using a settled wastewater inoculum and a 7-day static incubation followed by three weekly subcultures, an initial 4,6-dinitro-o-cresol concentration of 5 ppm was degraded 52, 58, 56, and 51% in the original, first, second, and third subcultures after 7 days, respectively(1). With an initial concentration of 10 ppm, degradation was 0, 5, 11, and 14% after 7 days for the original, first, second, and third subcultures, respectively(1). 4,6-Dinitro-o-cresol was considered difficult to degrade, <20% elimination, within the prescribed test period, with the Zahn-Wellens test(2). A theoretical BOD of 22.3% was measured in a Warburg respirometer over a 3 hr incubation period using an initial concentration of 100 ppm and a mixed bacteria culture adapted to phenol(3). Mixed bacteria cultures (primarily Pseudomonadaceae) obtained from mud, soil, and water degraded only 1% of initial 4,6-dinitro-o-cresol (207 ppm) in 48 hr static flask tests using mineral solutions and 4,6-dinitro-o-cresol as the only carbon source(4). An activated sludge system receiving an influent of 11 ppb 4,6-dinitro-o-cresol was able to degrade 99% of the compound(5). In neutral and mildly alkaline soils, doses of 10-150 ppm 4,6-dinitro-o-cresol increased CO₂ output by 10-30% over control, although there was a lag period before stimulation at concentrations above 50 ppm; in acidic soil, only low concentrations (1-20 ppm) produced significant stimulation(6). 4,6-Dinitro-o-cresol was found to increase CO₂ production from soil microflora at low concentrations, but decrease at high concentrations(7). Biodegradation half-lives of 4,6-dinitro-o-cresol in natural water were reported as 7 (aerobic) and 2.8 (anaerobic) days(8). No loss of 4,6-dinitro-o-cresol was observed when 4,6-dinitro-o-cresol was incubated in the dark with Texas soil (slightly basic sandy loam, 3.25% organic matter) and Mississippi soil (acidic soil, <1% organic matter) over a 65 day period(9). These soils had no previous exposure to industrial chemicals or wastes and did not receive any pre-treatment such as soil amendments or acclimated biological cultures(9). After a lag period of 80 days, 4,6-dinitro-o-cresol (25 ug/L) degraded quickly (rate constant 2.1 ug/L/day) under aerobic conditions in column

experiments using groundwater and sediment from a shallow, unconfined, aquifer near Vejen, Denmark(10). 4,6-Dinitro-o-cresol, present at 100 mg/L, reached 4% of its theoretical BOD in 4 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MTI test(11).

Bioaccumulative potential

BCF values of <0.3-0.7 at 50 ug/L and <2.9 at 5 ug/L were measured for carp after a 6 week exposure(1). Using bioaccumulation test OECD 305E, which is a dynamic flow-through test, the BCF for zebra fish (*Brachydanio rerio*) were calculated from the kinetics of the uptake and clearance phases and a BCF of 1.4 was found for 2,4-dinitro-o-cresol(2). BCF values ranging from 56-64 were found for *Pimephales promelas* (fathead minnow) after a 24-30 day exposure to 4,6-dinitro-o-cresol (0.6-7.8 ug/L)(3). A BCF of 1.5 was reported for fish(4). According to a classification scheme(5), these BCF values suggest the potential for bioconcentration in aquatic organisms is low to moderate(SRC).

Mobility in soil

Koc values for 4,6-dinitro-o-cresol derived from experimental measurements have been reported as 257(1) and 300(2). A Koc for 4,6-dinitro-o-cresol of 23 was reported for sandy loam(3). According to a classification scheme(4), these Koc values suggest that 4,6-dinitro-o-cresol is expected to have very high to moderate mobility in soil. The pKa of 4,6-dinitro-o-cresol is 4.31(5), indicating that this compound will exist partially in the anion form in the environment and anions generally do not adsorb more strongly to soils containing organic carbon and clay than their neutral counterparts(6). In an aquifer laboratory and field study in Denmark, 4,6-dinitro-o-cresol had Kd sorption coefficient values ranging from 0.10 to 0.98 with stronger sorption occurring at lower pHs where the neutral form of the compound was at a higher percentage than at the higher pHs(7); this indicates the anionic form of 4,6-dinitro-o-cresol is more mobile in soil than the neutral form(SRC).

Other adverse effects

no data available

SECTION 13: Disposal considerations

Disposal methods

Product

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

Contaminated packaging

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be

punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

SECTION 14: Transport information

UN Number

ADR/RID: UN3014 (For reference only, please check.)

IMDG: UN3014 (For reference only, please check.)

IATA: UN3014 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: SUBSTITUTED NITROPHENOL PESTICIDE, LIQUID, TOXIC (For reference only, please check.)

IMDG: SUBSTITUTED NITROPHENOL PESTICIDE, LIQUID, TOXIC (For reference only, please check.)

IATA: SUBSTITUTED NITROPHENOL PESTICIDE, LIQUID, TOXIC (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 6.1 (For reference only, please check.)

IMDG: 6.1 (For reference only, please check.)

IATA: 6.1 (For reference only, please check.)

Packing group, if applicable

ADR/RID: I (For reference only, please check.)

IMDG: I (For reference only, please check.)

IATA: I (For reference only, please check.)

Environmental hazards

ADR/RID: Yes

IMDG: Yes

IATA: Yes

Special precautions for user

no data available

Transport in bulk according to IMO instruments

no data available

SECTION 15: Regulatory information

Safety, health and environmental regulations specific for the product in question

European Inventory of Existing Commercial Chemical Substances (EINECS)

Listed.

EC Inventory

Listed.

United States Toxic Substances Control Act (TSCA) Inventory

Listed.

China Catalog of Hazardous chemicals 2015

Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Listed.

IECSC)

Listed.

Korea Existing Chemicals List (KECL)

Listed.

SECTION 16: Other information

Abbreviations and acronyms

CAS: Chemical Abstracts Service

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

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

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

References

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

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

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

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website: http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

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

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

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

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

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

Other Information

Do NOT take working clothes home. Technical grade may cause skin sensitization.

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any