

Chemical Safety Data Sheet MSDS / SDS

1-chloro-2,4-dinitrobenzene 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: 1-chloro-2,4-dinitrobenzene

CAS: 97-00-7

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

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

Acute toxicity - Category 4, Oral

Acute toxicity - Category 2, Dermal

Skin irritation, Category 2
Skin sensitization, Category 1
Serious eye damage, Category 1
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)

H302 Harmful if swallowed
H310 Fatal in contact with skin
H315 Causes skin irritation
H317 May cause an allergic skin reaction
H318 Causes serious eye damage
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.
P273 Avoid release to the environment.

Response

P301+P317 IF SWALLOWED: Get medical help.
P330 Rinse mouth.
P302+P352 IF ON SKIN: Wash with plenty of water/...
P316 Get emergency medical help immediately.
P321 Specific treatment (see ... on this label).
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.
P333+P317 If skin irritation or rash occurs: Get medical help.
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.
P391 Collect spillage.

Storage

P405 Store locked up.

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:	1-chloro-2,4-dinitrobenzene
Common names and synonyms:	1-chloro-2,4-dinitrobenzene
CAS number:	97-00-7
EC number:	202-551-4
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

Wear protective gloves when administering first aid. Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer immediately 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 one or two glasses of water to drink. Do NOT induce vomiting. Refer for medical attention .

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 153 [Substances - Toxic and/or Corrosive (Combustible)]: TOXIC; 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. Effects of contact or inhalation may be delayed. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may be corrosive and/or toxic and cause pollution. (ERG, 2016)

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. Nitrates, nitrites, and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

To fight fire use /carbon dioxide/, dry chemical.

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. Combat fire from a sheltered position.

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. Vacuum with specialist equipment (See Notes) or carefully sweep into 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. Vacuum with specialist equipment (See Notes) or carefully sweep into 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

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. NO contact with incompatible substances. See Chemical Dangers. Do NOT expose to friction or shock. 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

Fireproof. Separated from strong oxidants, strong bases, strong reducing agents, food and feedstuffs and ammonia. Store in an area without drain or sewer access. PROTECT AGAINST PHYSICAL DAMAGE, KEEP AWAY FROM HEAT AND SOURCES OF IGNITION OR ACUTE FIRE HAZARD AREAS. STORAGE AREA SHOULD BE EQUIPPED WITH AN AUTOMATIC SPRINKLER SYSTEM IF WITHIN A BUILDING.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

MAK sensitization of skin (SH)

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 face shield 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:	Solid.
Colour:	Yellow crystals
Odour:	Almond odor

Melting point/freezing point:	Ca. 50 °C.
Boiling point or initial boiling point and boiling range:	315 °C. Atm. press.:760 Torr.
Flammability:	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit:	Lower flammable limit: 2% by volume; Upper flammable limit: 22% by volume
Flash point:	194 °C. Atm. press.:760 Torr.
Auto-ignition temperature:	Ca. 432°C. Atm. press.:1 atm.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	13.8 [ug/mL]
Partition coefficient n-octanol/water:	log Pow = 2.24. Temperature:23.3 °C.
Vapour pressure:	0 Pa. Temperature:32 °C.;0 Pa. Temperature:40 °C.;0 Pa. Temperature:25 °C. Remarks:Extrapolated from log P versus 1/T.
Density and/or relative density:	1.68 g/cm ³ . Temperature:20 °C.
Relative vapour density:	6.98 (Air = 1)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

May decompose explosively on shock, friction or concussion. May explode on heating even in the absence of air. Reacts with strong oxidants and strong bases. Reacts violently with ammonia and strong reducing agents. This generates fire and explosion hazard. On combustion, forms toxic and corrosive gases and fumes including hydrogen chloride and nitrogen oxides.

Chemical stability

no data available

Possibility of hazardous reactions

Combustible when exposed to heat or flame. Self-reactive [Halpern, Chem. and Eng. News, 29:2666(1951)]. The mixture of this compound with hydrazine hydrate caused a violent reaction.

Conditions to avoid

no data available

Incompatible materials

Explosive reaction with ammonia at 170 deg C/40 bar.

Hazardous decomposition products

no data available

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male) - ca. 939 mg/kg bw.

Inhalation: no data available

Dermal: LD50 - rabbit (male) - ca. 130 mg/kg bw.

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 severely irritating to the skin and eyes. The substance may cause effects on the blood. This may result in the formation of methaemoglobin. Exposure to high concentrations could cause death.

STOT-repeated exposure

Repeated or prolonged contact may cause skin sensitization. The substance may have effects on the blood. This may result in a decrease in haemoglobin and a decrease of blood cells.

Aspiration hazard

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.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Danio rerio (previous name: Brachydanio rerio) - 0.71 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - 0.59 mg/L - 48 h.

Toxicity to algae: EC50 - Desmodesmus subspicatus (previous name: Scenedesmus subspicatus) - 0.392 mg/L - 72 h.

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: 1-Chloro-2,4-dinitrobenzene is reported as non-biodegradable in water based on an aqueous screening biodegradation test using 100 ppm as an initial concn, activated sludge inoculum and a 2 week incubation period(1). 1-Chloro-2,4-dinitrobenzene, present at 100 mg/L, reached 0 percent of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L and the Japanese MITI test suggesting the compound is not readily biodegradable(2). Structurally similar compounds have been shown to undergo biodegradation slowly in the environment(3,4). The half-life of 1-fluoro-2,4-dinitrobenzene in a dry silt loam soil was greater than 50 days(3) suggesting biodegradation of 1-chloro-2,4-dinitrobenzene also occurs slowly in the environment(SRC).

Bioaccumulative potential

The BCF in carp (Cyprinus carpio) ranged from <4.2 to <44 at test concentrations of 1-10 ppb 1-chloro-2,4-dinitrobenzene over a 6-week exposure period(1). According to a classification scheme(2), these BCF values suggest the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

A Koc of 501 was measured for 1-chloro-2,4-dinitrobenzene using a sediment (1.28% organic carbon content) collected from the Yangtse River in China(1). Sorption to montmorillonite clay is stronger (Koc of 6000)(2). Using a structure estimation method based on molecular connectivity indices(3), the Koc of 1-chloro-2,4-dinitrobenzene can be estimated to be 575(SRC). According to a classification scheme(4), Koc values of 501-575 suggests that 1-chloro-2,4-dinitrobenzene is expected to have low mobility in soil. It has been shown that nitrobenzenes adsorb strongly to clay surfaces and the mobility of 1-chloro-2,4-dinitrobenzene is expected to be low in soils rich in clay content(5,6).

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: UN3441 (For reference only, please check.)

IMDG: UN3441 (For reference only, please check.)

IATA: UN3441 (For reference only, please check.)

UN Proper Shipping Name

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

IMDG: CHLORODINITROBENZENES, SOLID (For reference only, please check.)

IATA: CHLORODINITROBENZENES, SOLID (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: II (For reference only, please check.)

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

IATA: II (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

NEVER use a domestic-type vacuum cleaner to vacuum the substance, only use specialist equipment.

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