Chemical Safety Data Sheet MSDS / SDS

1,4-dinitrobenzene SDS

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

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

Product identifier

Product name: 1,4-dinitrobenzene

CAS: 100-25-4

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

Acute toxicity - Category 2, Inhalation
Specific target organ toxicity – repeated exposure, 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
H330 Fatal if inhaled
H373 May cause damage to organs through prolonged or repeated exposure
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/...
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.
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.
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.

P320 Specific treatment is urgent (see ... on this label).
P319 Get medical help if you feel unwell.
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:	1,4-dinitrobenzene
Common names and synonyms:	1,4-dinitrobenzene
CAS number:	100-25-4
EC number:	202-833-7
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 and then wash skin with water and soap. 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

INHALATION OR INGESTION: Headache, vertigo, nausea, vomiting, diarrhea, fever, rapid weak pulse, decreased blood pressure, cyanosis, exhaustion, hepatomegaly, jaundice, albuminurea, hematuria, visual scotomata, amblyopia and nystagmus. EYES: Irritation. SKIN: Stains skin yellow; if skin contact is prolonged, can be absorbed into blood causing same symptoms as for inhalation. (USCG, 1999)

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

Basic treatment: Establish a patent airway. Suction if necessary. Watch for signs of respiratory insufficiency and assist ventilations if necessary. Administer oxygen by nonrebreather mask at 10 to 15 L/min. Monitor for shock and treat if necessary . Anticipate seizures and treat if necessary . For eye contamination, flush eyes immediately with water. Irrigate each eye continuously with normal saline during transport . Do not use emetics. For ingestion, rinse mouth and administer 5 ml/kg up to 200 ml of water for dilution if the patent can swallow, has a strong gag reflex, and does not drool. Administer activated charcoal . Aniline and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

For rescue purposes wear full protective clothing. Fight fire from an explosion-resistant location. In advanced or massive fires, area should be evacuated. If fire occurs in vicinity of this material water should be used to keep containers cool. 1,2-Dinitrobenzene

Specific hazards arising from the chemical

Special Hazards of Combustion Products: When heated to decomposition toxic fumes of oxides of nitrogen released. Behavior in Fire: Decomposes explosively. Can be detonated by shock or heat under confinement that will permit high pressure buildup (USCG, 1999)

Special protective actions for fire-fighters

Use water spray, foam, 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

Consult an expert! Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: complete protective clothing including self-contained breathing apparatus.

Environmental precautions

Consult an expert! Sweep spilled substance into covered containers. If appropriate, moisten first to prevent dusting. Carefully collect remainder. Then store and dispose of according to local regulations. Do NOT let this chemical enter the environment. Personal protection: complete protective clothing including self-contained breathing apparatus.

Methods and materials for containment and cleaning up

1. Remove all ignition sources. 2. Ventilate area of spill. 3. For small quantities, sweep onto paper or other suitable material and burn in suitable combustion chamber which allows burning in unconfined condition and is equipped with appropriate effluent gas cleaning device. Large quantities may be reclaimed; however, if this is not practical, dissolve in fuel oil and atomize in suitable combustion chamber equipped with cleaning an appropriate effluent gas cleaning device.

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. 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, strong bases, strong acids and food and feedstuffs. See Chemical Dangers.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.15 ppm as TWA; (skin); BEI issued.MAK: skin absorption (H); carcinogen category: 3B

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:	P-dinitrobenzene is a colorless to yellow solid. Sinks and mixes slowly with water. (USCG, 1999)
Colour:	White crystals
Odour:	no data available

Melting point/freezing point:	495°C(lit.)
Boiling point or initial boiling point and boiling range:	160°C/10mmHg(lit.)
Flammability:	Combustible Solid
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	96°C(lit.)
Auto-ignition temperature:	no data available
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= 1.46
Vapour pressure:	0.00206mmHg at 25°C
Density and/or relative density:	1.486g/cm3
Relative vapour density:	5.8 (air= 1 at boiling point of dinitrobenzene) /Dinitrobenzene, all isomers/
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

On combustion, forms toxic gases and fumes including nitrogen oxides. Reacts violently with strong oxidants, strong bases and metals (tin and zinc). This generates fire and explosion hazard. Mixtures with nitric acid are highly explosive.

Chemical stability

no data available

Possibility of hazardous reactions

Dust explosion possible if in powder or granular form, mixed with air.All three isomers have similar properties and may react vigorously with oxidizing materials. Their reaction with nitric acid (nitration) will lead to a mixture of trinitrobenzenes possessing high-explosive properties [Urbanski, 1967, vol. 3, p. 290]. If heat and reaction conditions of the nitration are not controlled, detonation comparable to TNT may occur [Anon., J. R. Inst. Chem., 1960, 84, p. 451]. Mixture of 1,3-dinitrobenzene with tetranitromethane was found highly explosive [Urbanski, 1964, vol. 1, 592]. 1,2-dinitrobenzene is a severe explosion hazard when shocked or exposed to heat or flame. When heated to decomposition all dinitrobenzens emit toxic fumes of nitrogen oxides [Sax, 9th ed., 1996, p. 1374].

Conditions to avoid

no data available

Incompatible materials

Contact with strong oxidizers may cause fires & explosions. Contact with caustics & metals such as tin & zinc may cause evolution of heat & incr in pressure.

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

Oral: no data available

Inhalation: no data available

Dermal: no data available

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 irritating to the eyes and respiratory tract. The substance may cause effects on the blood. This may result in the formation of methaemoglobin. The effects may be delayed. Medical observation is indicated.

STOT-repeated exposure

The substance may have effects on the blood. This may result in anaemia. The substance may have effects on the liver. This may result in liver impairment.

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 Pimephales promelas (fathead minnow) 0.687 (0.642-0.734) mg/l 24 hr, wt 164 mg, flow-through bioassay, dissolved oxygen 7.4 (4.6-8.8) mg/l, water hardness 44.9 (42.4-46.6) mg/l as CaCO3, pH 6.9-7.7, alkalinity 42.9 (39.6-61.4) mg/l CaCO3, temp: 26.4 +/- 1.4 deg C, Purity 98%

Toxicity to daphnia and other aquatic invertebrates: no data available

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

More than 64 days were required to achieve a total loss of 1,4-dinitrobenzene when incubated with Niagara silt loam inoculum at 25 deg C(1). No additional data were available concerning 1,4-dinitrobenzene, but 1,2-dinitrobenzene and 1,3-dinitrobenzene are degraded to aromatic amines and ring opened species upon anaerobic and aerobic incubation, respectively, with sewage effluent(2). Dinitrobenzene (isomer not specified), 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(3), suggesting biodegradation occurs slowly(SRC).

Bioaccumulative potential

A BCF value of 5 was measured for 1,4-dinitrobenzene in fish(1). BCF values of 2-38 were measured in carp exposed to dinitrobenzene (isomer not specified) over a 6 week incubation period(2). According to a classification scheme(3), this BCF value suggest bioconcentration in aquatic organisms is low to moderate(SRC).

Mobility in soil

The Koc of 1,4-dinitrobenzene is estimated as 150(SRC), using a measured log Kow of 1.46(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,4-dinitrobenzene is expected to have high mobility in soil. It has been shown that nitrophenols and nitrobenzenes adsorb strongly to clay through an interaction between the nitro group and the water molecules or metallic cations in the clay(4), and 1,4-dinitrobenzene is expected to similarly bind to clays(SRC). The adsorption of 1,4-dinitrobenzene was studied in monmorillonite, kaolinite and illite clays(5). Adsorption coefficients (Kd) of 188, 1,460 and 3,100 L/kg were measured in kaolinite, illite and monmorillonite, respectively(5).

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: UN3443 (For reference only, please check.)
IMDG: UN3443 (For reference only, please check.)
IATA: UN3443 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: DINITROBENZENES, SOLID (For reference only, please check.)
IMDG: DINITROBENZENES, SOLID (For reference only, please check.)
IATA: DINITROBENZENES, 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

Use of alcoholic beverages enhances the harmful effect. Depending on the degree of exposure, periodic medical examination is suggested. Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available. See ICSCs 0460, 0691 and 0725. NFPA Code: H3; F1; R4; for 1,2-Dinitrobenzene.