

## Chemical Safety Data Sheet MSDS / SDS

## 1,3-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: 1,3-dinitrobenzene  
CAS: 99-65-0

**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  
Telephone: +91 9550333722

**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:	1,3-dinitrobenzene
Common names and synonyms:	1,3-dinitrobenzene
CAS number:	99-65-0
EC number:	202-776-8
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**

Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: Highly toxic, may be fatal if inhaled, swallowed or absorbed through skin. 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)

Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: Highly toxic, may be fatal if inhaled, swallowed or absorbed through skin. 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)

Inhalation or ingestion causes loss of color, nausea, headache, dizziness, drowsiness, and collapse. Eyes are irritated by liquid. Stains skin yellow; if contact is prolonged, can be absorbed into blood and cause 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 patient 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**

Fire Fighting Respirator: Self-contained breathing apparatus with a full facepiece operated in pressure-demand or other positive pressure mode.

### **Specific hazards arising from the chemical**

Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: Combustible material: may burn but does not ignite readily.

Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)  
Excerpt from ERG Guide 152 [Substances - Toxic (Combustible)]: Combustible material: may burn but does not ignite readily.  
Containers may explode when heated. Runoff may pollute waterways. Substance may be transported in a molten form. (ERG, 2016)  
Behavior in Fire: May explode (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 & burn in a suitable combustion chamber which allows burning in an unconfined condition & is equipped with an appropriate effluent gas cleaning device. Large quantities may be reclaimed; however, if this is not practical, dissolve in fuel oil & atomize in a suitable combustion chamber equipped with 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 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:	One or more of the three isomeric (1,2- 1,3- and 1,4-) dinitrobenzenes, which are solids at room conditions, presumably in a non-aqueous solvent or carrier. Toxic by skin absorption. Exposure of the confined material to heat or shock may result in explosive decomposition. Produces toxic oxides of nitrogen during combustion.
Colour:	Yellowish crystals
Odour:	no data available
Melting point/freezing point:	-61°C(lit.)
Boiling point or initial boiling point and boiling range:	297°C(lit.)
Flammability:	Combustible Solid
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	150°C
Auto-ignition temperature:	470°C
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	0.02 % (NIOSH, 2016)
Partition coefficient n-octanol/water:	log Kow= 1.49
Vapour pressure:	2X10 <sup>-4</sup> mm Hg @ 25 deg C
Density and/or relative density:	1.368g/mLat 25°C(lit.)

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

May explode on heating even in the absence of air. On combustion, forms toxic gases and fumes including nitrogen oxides. Reacts violently with strong oxidants, strong bases and reducing metals (tin and zinc). This generates fire and explosion hazard. Attacks some plastics and rubber.

May explode on heating even in the absence of air. Reacts violently with powdered metals and strong oxidants. This generates fire and explosion hazard. Decomposes on heating. This produces toxic fumes including nitrogen oxides.

### Chemical stability

no data available

### Possibility of hazardous reactions

Combustible Dust explosion possible if in powder or granular form, mixed with air., Dust explosion possible if in powder or granular form, mixed with air. DINITROBENZENE SOLUTION may react vigorously with oxidizing materials. Reaction with nitric acid (nitration) leads 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 that of TNT may occur [Anon., J. R. Inst. Chem., 1960, 84, p. 451]. A mixture of 1,3-dinitrobenzene with tetranitromethane can be highly explosive [Urbanski, 1964, vol. 1, 592]. 1,2-dinitrobenzene is a severe explosion hazard when shocked or exposed to heat or flame.

### Conditions to avoid

no data available

### Incompatible materials

Mixture with nitric acid is a high explosive. Mixture with tetranitromethane is a high explosive very sensitive to sparks.

### Hazardous decomposition products

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



## SECTION 11: Toxicological information

### Acute toxicity

Oral: LD50 Rat oral as a 1% suspension in corn oil 83 mg/kg with fiducial limits 56-124 mg/kg

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

CLASSIFICATION: D; not classifiable as to human carcinogenicity. BASIS FOR CLASSIFICATION: Based on no data in humans and animals. HUMAN CARCINOGENICITY DATA: None. ANIMAL CARCINOGENICITY DATA: None.

### 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. The substance may have effects on the nervous system. Animal tests show that this substance possibly causes toxicity to human reproduction or development. May cause impaired vision.

### **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: no data available

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**

Anaerobic and aerobic incubation of 1,3-dinitrobenzene with sewage effluent at 29 deg C resulted in about 85% and 40% degradation after 28 days, respectively(1). The products of the anaerobic incubations were aromatic amines while under aerobic conditions, ring cleavage and possible mineralization of 1,3-dinitrobenzene occurred(1). More than 64 days were required to achieve a total loss of 1,3-dinitrobenzene when incubated with Niagara silt loam inoculum at 25 deg C(2). Microorganisms isolated from the Tennessee River near a munitions production facility were shown to biodegrade 1,3-dinitrobenzene(3). At  $1 \times 10^6$  microorganisms/mL and 25 deg C, the half-life of 1,3-dinitrobenzene in river water samples and enrichment cultures were 1 and 9.7 days, respectively(3). However, 1,3-dinitrobenzene did not biodegrade in pristine river and creek water from Maryland, suggesting that microbial adaptation is necessary for degradation to occur(3). After 3 hr incubation at 30 deg C with phenol adapted bacteria from soil and related environments, 75% of the initial amount of 1,3-dinitrobenzene was degraded(4). 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(5), suggesting biodegradation occurs slowly(SRC).

### **Bioaccumulative potential**

A BCF value of 75 was measured for 1,3-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 1,3-dinitrobenzene is estimated as 150(SRC), using a measured log Kow of 1.49(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,3-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 1,3-dinitrobenzene is expected to similarly bind to clays(SRC). The adsorption of 1,3-dinitrobenzene was studied in montmorillonite, clay and an adsorption coefficient of 4,500 L/kg was measured(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](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, 0692 and 0725. NFPA Code: H3; F1; R4; for 1,2-Dinitrobenzene.

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