Chemical Safety Data Sheet MSDS / SDS

1,3,5-trinitrobenzene 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: 1,3,5-trinitrobenzene

CAS: 99-35-4

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

Explosives, Division 1.1
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)

H201 Explosive; mass explosion hazard
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

P210 Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.
P230 Keep wetted with ...
P234 Keep only in original packaging.
P240 Ground and bond container and receiving equipment.
P250 Do not subject to grinding/shock/friction/....
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...
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.
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

P370+P372+P380+P373 In case of fire: Explosion risk. Evacuate area. DO NOT fight fire when fire reaches explosives.
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

P401 Store in accordance with...
P405 Store locked up.
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

Disposal

P503 Refer to manufacturer/supplier... for information on disposal/recovery/recycling.
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:	1,3,5-trinitrobenzene
Common names and synonyms:	1,3,5-trinitrobenzene
CAS number:	99-35-4
EC number:	202-752-7
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Some are toxic and may be fatal if inhaled, swallowed or absorbed through skin. Contact may cause burns to skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)
Excerpt from ERG Guide 112 [Explosives* - Division 1.1, 1.2, 1.3 or 1.5]: Fire may produce irritating, corrosive and/or toxic gases. (ERG, 2016)
Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Some are toxic and may be fatal if inhaled, swallowed or absorbed through skin. Contact may cause burns to skin and eyes. Fire may produce irritating, corrosive and/or toxic gases. Runoff from fire control or dilution water may cause pollution. (ERG, 2016)

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

Basic treatment: Establish a patent airway (oropharyngeal or nasopharyngeal airway, if needed). 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 pulmonary edema and treat if necessary . 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 0.9% saline (NS) 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 . Aromatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Suitable extinguishing media

If material on fire or involved in fire: Dangerously explosive. Do not fight fires in a cargo of explosives. Evacuate area and let burn. Trinitrobenzene

Specific hazards arising from the chemical

Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Flammable/combustible material. May be ignited by heat, sparks or flames. DRIED OUT material may explode if exposed to heat, flame, friction or shock; treat as an explosive, refer to ERG Guide 112. Keep material wet with water or treat as an explosive, refer to ERG Guide 112. Runoff to sewer may create fire or explosion hazard. (ERG, 2016)
Excerpt from ERG Guide 112 [Explosives* - Division 1.1, 1.2, 1.3 or 1.5]: MAY EXPLODE AND THROW FRAGMENTS 1600 METERS (1 MILE) OR MORE IF FIRE REACHES CARGO. For information on "Compatibility Group" letters, refer to Glossary section. (ERG, 2016)
Excerpt from ERG Guide 113 [Flammable Solids - Toxic (Wet/Desensitized Explosive)]: Flammable/combustible material. May be ignited by heat, sparks or flames. DRIED OUT material may explode if exposed to heat, flame, friction or shock; treat as an explosive, refer to ERG Guide 112. Keep material wet with water or treat as an explosive, refer to ERG Guide 112. Runoff to sewer may create fire or explosion hazard. (ERG, 2016)

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours.Avoid contacting with skin and eye. Use personal protective equipment.Wear chemical impermeable gloves. Ensure adequate ventilation.Remove all sources of ignition. Evacuate personnel to safe areas.Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

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

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Trinitrobenzene, wetted with not less than 30% water is a light yellow crystalline sludge or slurry. Burns but may require some effort to ignite. A high explosive when dry. Easily ignited and burns very vigorously when dry. Insoluble in water. Produces toxic oxides of nitrogen during combustion.
Colour:	Yellow crystals
Odour:	no data available
Melting point/freezing point:	-23°C(lit.)
Boiling point or initial boiling point and boiling range:	138°C
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	34°C(lit.)
Auto-ignition temperature:	no data available
Decomposition temperature:	no data available

pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Soluble in alcohol and ether
Partition coefficient n-octanol/water:	log Kow = 1.18
Vapour pressure:	6.44X10-6 mm Hg at 25 deg C (extrapolated)
Density and/or relative density:	1.705g/cm3
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

no data available

Possibility of hazardous reactions

Aromatic nitro compounds, such as TRINITROBENZENE, range from slight to strong oxidizing agents. If mixed with reducing agents, including hydrides, sulfides and nitrides, they may begin a vigorous reaction that culminates in a detonation. The aromatic nitro compounds may explode in the presence of a base such as sodium hydroxide or potassium hydroxide even in the presence of water or organic solvents. The explosive tendencies of aromatic nitro compounds are increased by the presence of multiple nitro groups.

Conditions to avoid

no data available

Incompatible materials

The product /potassium 4-methyoxy-1-aci-nitro-3,5-dinitro-2,5-cyclohexadienonide/ of interaction of /1,3,5-/trinitrobenzene and concn aqueous potassium hydroxide in methanol is explosive, and analyses as the hemihydrate of a hemiacetal of the aci-p-quinonoid form of picric acid, and/or the mesomeric o-forms.

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 Guinea pig oral 730 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

no data available

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: Pimephales promelas (Fathead minnow); Conditions: freshwater; static; Concentration: 1030 ug/L for 96 hr /formulated product

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater; static; Concentration: 2700 ug/L for 48 hr; Effect: intoxication, immobile /formulated product

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: The microbial degradation of 1,3,5-trinitrobenzene was incomplete and unsustained in Tennessee river water(1). Nitro group reduction occurred in the presence of added nutrients and lab cultures of Tennessee river microorganisms(1). Simulated biological treatment system, consisting of an aerator inoculated with A. agilis (first stage) and an activated sludge system (2nd stage), initial concn 118-146 mg/L nitroaromatic compounds, 96-98% removal in first stage and 2-4% removal in second stage(2). 1,3,5-Trinitrobenzene at an initial concn of 100 ppm was found to be resistant to biodegradation when incubated 180 minutes in a Warburg respirometer inoculated with a phenol-adapted mixed culture of microorganisms obtained from garden soil, compost, river sediment, and a petroleum refinery waste lagoon(3). 1,3,5-Trinitrobenzene was reported to degrade 84% in 7 days from surface water at room temperature(4). 1,3,5-Trinitrobenzene was degraded an average of 93.5% in 3 days at room temperature in three different soils; Windsor (pH 6.2, clay 30 %, total organic carbon 1.1%), Charlton (pH 6.0, clay 20%, total organic carbon 1.8%), Ft Edwards (pH 8.4, clay 70%, total organic carbon 0.5%)(5).

Bioaccumulative potential

An estimated BCF of 1.6 was calculated in fish for 1,3,5-trinitrobenzene(SRC), using a log Kow of 1.18(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

The Koc of 1,3,5-trinitrobenzene is estimated as 104(SRC), using a log Kow of 1.18(1) and a regression-derived equation(2). According to a classification scheme(3), this estimated Koc value suggests that 1,3,5-trinitrobenzene is expected to have high mobility in soil.

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: UN0214 (For reference only, please check.)
IMDG: UN0214 (For reference only, please check.)
IATA: UN0214 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: TRINITROBENZENE, dry or wetted with less than 30% water, by mass? (For reference only, please check.)
IMDG: TRINITROBENZENE, dry or wetted with less than 30% water, by mass? (For reference only, please check.)
IATA: TRINITROBENZENE, dry or wetted with less than 30% water, by mass? (For reference only, please check.)

Transport hazard class(es)

ADR/RID: 1.1D (For reference only, please check.)
IMDG: 1.1D (For reference only, please check.)
IATA: 1.1D (For reference only, please check.)

Packing group, if applicable

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

Not Listed.

(PICCS)

Listed.

Vietnam National Chemical Inventory

Not Listed.

IECSC)

Not Listed.

Korea Existing Chemicals List (KECL)

Not 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/