Chemical Safety Data Sheet MSDS / SDS

DINITROTOLUENE

Revision Date: 2024-12-21 Revision Number: 1

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

Product identifier

Product name : DINITROTOLUENE

CBnumber : CB1233252

CAS : 25321-14-6

EINECS Number : 246-836-1

Synonyms : DINITROTOLUENE, dinitrotoluenes

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

Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing

Telephone : 010-86108875

SECTION 2: Hazards identification

Classification of the substance or mixture

Acute toxicity - Category 3, Oral

Acute toxicity - Category 3, Dermal

Acute toxicity - Category 3, Inhalation

Germ cell mutagenicity, Category 2

Carcinogenicity, Category 1B

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

Reproductive toxicity, Category 2

Label elements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H301 Toxic if swallowed

H311 Toxic in contact with skin

H331 Toxic if inhaled

H341 Suspected of causing genetic defects

H350 May cause cancer

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.

P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P271 Use only outdoors or in a well-ventilated area.

P203 Obtain, read and follow all safety instructions before use.

P260 Do not breathe dust/fume/gas/mist/vapours/spray.

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.

P318 IF exposed or concerned, get medical advice.

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

no data available

SECTION 3: Composition/information on ingredients

Substance

Product name : DINITROTOLUENE

Synonyms : DINITROTOLUENE, dinitrotoluenes

CAS : 25321-14-6
EC number : 246-836-1
MF : C7H6N2O4
MW : 182.134

SECTION 4: First aid measures

Description of 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 one or two glasses of water to drink. Refer for medical attention .

Most important symptoms and effects, both 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)

Ingestion or overexposure to vapors from hot liquid can cause loss of color, nausea, headache, dizziness, drowsiness, collapse. Hot liquid can burn eyes and skin. Prolonged skin contact with solid can give same symptoms as after inhalation or ingestion. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

In case of ingestion, induction of emesis is not recommended because of the potential for central nervous system depression. Gastric lavage and administration of activated charcoal may be considered soon after ingestion, provided airways are protected. Dinitrotoluene

SECTION 5: Firefighting measures

Extinguishing media

Water, dry chemical, or carbon dioxide from protected location.

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)

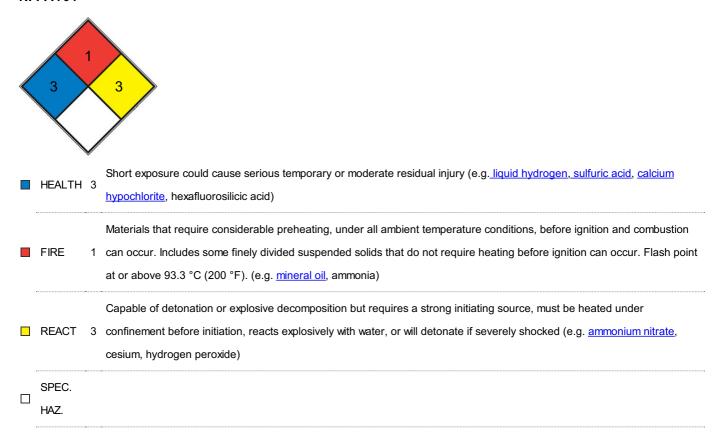
Special Hazards of Combustion Products: Nitrogen oxides and dense black smoke are produced in a fire. Behavior in Fire: Decomposition is self- sustaining at 280°C. Containers may explode in a fire. (USCG, 1999)

Advice for firefighters

Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water. Combat fire from a sheltered Chemical Book

position.

NFPA 704



SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. 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.

Environmental precautions

Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. 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.

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 suitable combustion chamber which allows burning in unconfined condition & is equipped with appropriate effluent gas cleaning device. large quantities may be reclaimed; ... if ... not practical, dissolve in fuel oil & atomize in suitable combustion chamber equipped with 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

Fireproof. Separated from strong bases, food and feedstuffs, oxidants and strong reducing agents. Well closed. Keep in a well-ventilated room. Store in an area without drain or sewer access.PRECAUTIONS FOR "CARCINOGENS": Storage site should be as close as practical to lab in which carcinogens are to be used, so that only small quantities required for ... expt need to be carried. Carcinogens should be kept in only one section of cupboard, an explosion-proof refrigerator or freezer (depending on chemicophysical properties ...) that bears appropriate label. An inventory ... should be kept, showing quantity of carcinogen & date it was acquired ... Facilities for dispensing ... should be contiguous to storage area. Chemical Carcinogens

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 0.2 mg/m3, as TWA; (skin); A3 (confirmed animal carcinogen with unknown relevance to humans); BEI issued.MAK: skin absorption (H); carcinogen category: 2

Biological limit values

no data available

Exposure controls

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

Individual protection measures

Eye/face protection

Wear safety goggles.

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

Information on basic physicochemical properties

| Physical state | Yellow crystals |
|----------------|-------------------------------------|
| Colour | Yellow needles or monoclinic prisms |
| Odour | SLIGHT ODOR |

| Melting point/freezing point | 65 - 90°C |
|--|---|
| Boiling point or initial boiling point and | 250 - 300°C |
| boiling range | |
| Flammability | Combustible Solid, but difficult to ignite. |
| Lower and upper explosion | no data available |
| limit/flammability limit | |
| Flash point | 207°C |
| Auto-ignition temperature | 400°C |
| Decomposition temperature | 250-300°C |
| рН | no data available |
| Kinematic viscosity | 0.0034553 Pa.s at 342.65 deg K |
| Solubility | Very slightly soluble (NTP, 1992) |
| Partition coefficient n-octanol/water | log Kow = 1.98 |
| Vapour pressure | 3.93E-05mmHg at 25°C |
| Density and/or relative density | 1.407 g/cm3 |
| Relative vapour density | 6.3 (NTP, 1992) (Relative to Air) |
| Particle characteristics | no data available |
| | |

SECTION 10: Stability and reactivity

Reactivity

NIOSH considers dinitrotoluene to be a potential occupational carcinogen. [50 mg/cu m] Dinitrotoluene

Heating may cause violent combustion or explosion. Decomposes on heating. This produces toxic and corrosive fumes including nitrogen oxides even in the absence of air. Reacts with reducing agents, strong bases and oxidants. This generates fire and explosion hazard. May explode on heating. Decomposes on heating. This produces toxic and corrosive fumes including nitrogen oxides even in the absence of air. Reacts with reducing agents, strong bases and oxidants. This generates explosion hazard.

Chemical stability

no data available

Possibility of hazardous reactions

Dust explosion possible if in powder or granular form, mixed with air., Dust explosion possible if in powder or granular form, mixed with air. DINITROTOLUENE is incompatible with strong oxidizing agents, caustics, active metals, tin and zinc (NTP, 1992). Decomposes at 250°C. Prolonged heating below this temperature causes some decomposition, and the presence of impurities may decrease the decomposition temperatures. Decomposition is self-sustaining at 280°C. Containers may explode in a fire (USCG, 1999). Reacts with oxidizing agents, caustics, nitric acid, reducing materials and metals such as zinc or tin. May react violently in the presence of a base or when heated to the boiling point. Attacks some forms of plastics, rubbers and coatings. (NTP, 1992).

Conditions to avoid

no data available

Incompatible materials

Dinitrotoluene held at 210 deg C (rather than 125 deg C as intended) for 10 days in a 50 mm steam heated transfer pipeline exploded.

Chemical Book

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Subsequent tests showed decomposition at 210 deg C (producing a significant pressure rise) in 1 day, and presence of sodium carbonate (but not rust) reduced the induction period. A maximum handling temperature of 150 deg C was recommended, (when the induction period was 32 days, or 14 days for alkali contaminated material).

Hazardous decomposition products

Spontaneously decomposes above 536 deg F (280 deg C) and will cause an explosive if confined. ... Air or oxygen is not required for decomposition or oxidation.

SECTION 11: Toxicological information

Acute toxicity

• Oral: LD50 Mouse oral 1630 mg/kg bw

Inhalation: no data availableDermal: 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

Evaluation: There is inadequate evidence in humans for the carcinogenicity of 2,4-dinitrotoluene. ... There is sufficient evidence in experimental animals for the carcinogenicity of 2,4-dinitrotoluene. ... Overall evaluation: 2,4-Dinitrotoluene ... /is/ possibly carcinogenic to humans (Group 2B).

Reproductive toxicity

A significant reduction in sperm counts and normal sperm morphology was observed in one study of chronically exposed workers while several other studies did not report these effects. A small, but statistically significant, increase in spontaneous abortions was reported in one study of chronically exposed workers; several methodological problems with the study were noted. In animals orally exposed to 2,4-dinitrotoluene, decreased fertility was reported. Decreased sperm production, testicular atrophy, and degenerated seminiferous tubules were observed in males, and ovarian atrophy and dysfunction were observed in female rats. No birth defects were observed in the offspring of animals fed 2,4-dinitrotoluene in the diet.

STOT-single exposure

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 the formation of methaemoglobin. This substance is possibly carcinogenic to humans. Animal tests show that this substance possibly causes toxicity to human reproduction or development.

Aspiration hazard

Evaporation at 20°C is negligible; a harmful concentration of airborne particles can, however, be reached quickly when dispersed, especially if powdered.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: Pimephales promelas (fathead minnow); Concentration: 24.3 mg/L for 96 hr (confidence limit 23.0 to 25.6 mg/L). Affected fish lost schooling behavior, were hypoactive and underreactive to external stimuli, swam near the tank surface and had increased respiration. They also had rigid musculature, convulsions and spinal column deformities. In addition, the fish were darkly colored and lost equilibrium prior to death. /Conditions of bioassay not specified

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water flea); Conditions: freshwater, renewal, 25 deg C, pH >7; Concentration: 38000 ug/L for 24 hr; Effect: behavior, equilibrium /formulation

Toxicity to algae: EC50; Species: Pseudokirchneriella subcapitata (Green Algae) exponential growth phase; Conditions: freshwater, static, 25 deg C, pH 6.0-7.5; Concentration: 14.3 uM for 96 hr (95% confidence interval: 10.5-19.2 uM); Effect: decreased population abundance Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: 2,4-Dinitrotoluene was reduced by 80%, of which 22% was transformed to 4-amino-2-nitrotoluene and 6% to 2-amino-4-nitrotoluene, by a mixture of microorganisms indigenous to an aquifer which underlies an explosives contaminated site(1); in the same study, approximately 28% of the 2,4-dinitrotoluene was mineralized to carbon dioxide within 28 days, while approximately 20% was not degraded within 28 days(1). In a wastewater treatment plant handling munitions wastewater, aerobic biodegradation of 2,4-dinitrotoluene was accelerated by addition of ethanol and phosphate(2); 4-amino-2-nitrotoluene and 2-amino-4-nitrotoluene were consistently observed as the main biodegradation reduction products(2). 2,4-Dinitrotoluene, present at 100 mg/L, reached 0% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test that suggests the compound is not readily biodegradable(3). In soil column studies using a munitions plant soil previously exposed to 2,4-nitrotoluene, 2,4-nitrotoluene biodegradation of 2,4-dinitrotoluene was rapid in the presence of natural mineral water, but slower in the presence of deionized water(4).

Bioaccumulative potential

Bioconcentration factor (weighted average) = 3.8 (calculated) for aquatic organisms that contain about 7.6% lipids.

Mobility in soil

In a loamy sand soil containing an organic matter content of 8.5 g/kg, 2,4-dinitrotoluene had measured Kd adsorption coefficients ranging from 0.28 to 1.11 cu cm/g(1) that correspond to a Koc range of 57 to 225(SRC). In three Chinese soils (organic carbon content of 0.47, 1.0 and 2.2%), measured Freundlich coefficients (Kf) for 2,4-dinitrotoluene ranged from 0.66 to 5.1 mmol-L/kg(2) that correspond to a Koc range of approximately 200 to 1000(SRC). Using a structure estimation method based on molecular connectivity indices(3), the Koc for 2,4-dinitrotoluene can be estimated to be 575(SRC). According to a classification scheme(4), a Koc range of 57-1000 suggests that 2,4-dinitrotoluene can have a high to low mobility range in soil. Leaching of 2,4-dinitrotoluene has been observed in soil column transport studies(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: UN3454 (For reference only, please check.)

IMDG: UN3454 (For reference only, please check.)

IATA: UN3454 (For reference only, please check.)

UN Proper Shipping Name

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

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

IATA: DINITROTOLUENES, 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

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

Not 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

ChemlDplus, 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

Commercial grades of DNT typically consist of a mixture of all 6 isomers, but mainly 2,4-DNT(78%) and 2,6-DNT (19%). Other UN-number: 1600 (molten). 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. Do NOT take working clothes home. See ICSCs 0727 and 0728.

Disclaimer

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.