

Chemical Safety Data Sheet MSDS / SDS

3,4-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 : 3,4-DINITROTOLUENE
CBnumber : CB5293157
CAS : 610-39-9
EINECS Number : 210-222-1
Synonyms : 4-methyl-1,2-dinitrobenzene,3,4-Dinitrotoluene

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 : 400-158-6606

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, long-term (Chronic) - Category Chronic 2
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

H411 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 : 3,4-DINITROTOLUENE

Synonyms : 4-methyl-1,2-dinitrobenzene,3,4-Dinitrotoluene

CAS	: 610-39-9
EC number	: 210-222-1
MF	: C7H6N2O4
MW	: 182.13

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

INHALATION, INGESTION OR SKIN ABSORPTION: Headache, weakness, nausea or dizziness, cyanosis, drowsiness, shortness of breath and collapse. EYES AND SKIN: Can burn eyes and skin. (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

Fire extinguishing agents: Water, carbon dioxide, or dry chemical.

Specific Hazards Arising from the Chemical

Special Hazards of Combustion Products: Emits toxic fumes of oxides of nitrogen. Behavior in Fire: May explode when exposed to heat or flame. (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 position.

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
Chemical Book

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. dinitrotoluene

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. Normally stored as a molten liquid. Separate from strong oxidizers & reducing agents. Hot water coils should not exceed 194 deg F (90 deg C). Dinitrotoluenes

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

Component	3,4-dinitrotoluene			
CAS No.	610-39-9			
	Limit value - Eight hours		Limit value - Short term	
	ppm	mg/m ³	ppm	mg/m ³
Austria	?	1,5	?	6
Denmark	?	0,15	?	0,3
Finland	?	0,2	?	?
Latvia	?	1	?	?
	Remarks			
Austria	TRK value (based on technical feasibility)			

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 risk-elimination area.

Individual protection measures

Eye/face protection

Wear safety goggles.

Skin protection

Protective gloves.

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	3,4-dinitrotoluene is a yellow to red solid or heated liquid with a slight odor. Solidifies in cool water. Solid and liquid sink in water . (USCG, 1999)
Colour	Yellow needles from carbon disulfide
Odour	Slight odor
Melting point/freezing point	54-57°C(lit.)
Boiling point or initial boiling point and boiling range	350.8°C at 760 mmHg
Flammability	Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
Lower and upper explosion limit/flammability limit	no data available
Flash point	>230 °F
Auto-ignition temperature	no data available
Decomposition temperature	250-300°C
pH	no data available
Kinematic viscosity	no data available
Solubility	Soluble in ethanol and carbon disulfide; slightly soluble in chloroform
Partition coefficient n-octanol/water	log Kow = 2.08
Vapour pressure	3.50X10 ⁻⁴ mm Hg at 25 deg C /extrapolated/
Density and/or relative density	1.407g/cm ³
Relative vapour density	6.28 (Air = 1)
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

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

Combustible material. Dust explosion possible if in powder or granular form, mixed with air. 3,4-DINITROTOLUENE may explode when exposed to heat or flame (USCG, 1999).

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

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

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 Rat oral 807 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

A3; Confirmed animal carcinogen with unknown relevance to humans. Dinitrotoluene

Reproductive toxicity

no data available

STOT-single exposure

The substance is mildly irritating to the skin. 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.

Aspiration hazard

A harmful concentration of airborne particles can be reached quickly when dispersed, especially if powdered.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50; Species: Pimephales promelas (Fathead Minnow) juvenile; Conditions: freshwater, static, 20 deg C, pH 7.2-8.6, hardness 26 mg/L CaCO₃, alkalinity 45 mg/L CaCO₃, dissolved oxygen 7.2 (6.8-8.5) mg/L; Concentration: 1500 ug/L for 96 hr /formulation
Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water Flea) 1st instar larva; Conditions: freshwater, static, 20 deg C, pH 7.2-8.6, hardness 26 mg/L CaCO₃, alkalinity 45 mg/L CaCO₃, dissolved oxygen 8.8 mg/L; Concentration: 3100 ug/L for 48 hr; Effect: intoxication, immobilization /formulation

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: 3,4-Dinitrotoluene was not mineralized in water from a pond and from Waconda Bay; however, 3,4-dinitrotoluene was co-metabolized when 500 ppm of yeast extract was added to the water from these two sources(1). The rate of degradation with added yeast extract in Searsville Pond water was $6.1 \times 10^{+10}$ mL/cell-hour, and in Waconda Bay water $0.89 \times 10^{+10}$ mL/cell-hour(1). 3,4-Dinitrotoluene, present at 100 mg/L, reached 0% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L and the Japanese MITI test(2).

Bioaccumulative potential

The BCF of 3,4-dinitrotoluene in carp (*Cyprinus carpio*) over a 6-week period was determined to be less than 0.27 and less than 2.7 when exposed to concentrations of 10 and 1 mg/L, respectively(1). According to a classification scheme(2), these BCF values suggest the potential for bioconcentration in aquatic organisms is low.

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 3,4-dinitrotoluene can be estimated to be 575(SRC). Using a structure estimation method based on a log Kow of 2.08(2), the Koc of 3,4-dinitrotoluene can be estimated to be 326(SRC). According to a classification scheme(3), these estimated Koc values suggest that 3,4-dinitrotoluene is expected to have medium to low 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: 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

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

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

PICCS

Not Listed.

Vietnam National Chemical Inventory

Listed.

IECSC

Not 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

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. UN number for molten form: UN1600, TEC (R) 61GT1-II.

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.