ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

3,5-dinitrotoluene

Revision Date:2023-05-06 Revision Number:1

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

Product identifier

Product name	: 3,5-dinitrotoluene
CBnumber	: CB8906726
CAS	: 618-85-9
EINECS Number	: 210-566-2
Synonyms	: 1-methyl-3,5-dinitrobenzene,BENZENE, 1-METHYL-3,5-DINITRO-

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 3

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

H412 Harmful 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.

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	: 3,5-dinitrotoluene
Synonyms	: 1-methyl-3,5-dinitrobenzene,BENZENE, 1-METHYL-3,5-DINITRO-
CAS	: 618-85-9

EC number	: 210-566-2
MF	: C7H6N2O4
MW	: 182.13

SECTION 4: First aid measures

Description of 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 and effects, both acute and delayed

no data available

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

Apply/ water, dry chemical, or carbon dioxide from protected location.

Specific Hazards Arising from the Chemical

no data available

Advice for firefighters

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

Environmental considerations - water spill: Use natural deep water pockets, excavated lagoons, or sand bag barriers to trap material at bottom. Remove trapped material with suction hoses. If dissolved, in region of 10 ppm or greater concentration, apply activated carbon at ten times the spilled amount. Use mechanical dredges or lifts to remove immobilized masses of pollutants and precipitates. Dinitrotoluene, liquid; dinitrotoluene, solid

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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

Component	3,5-dinitrotoluene			
CAS No.	618-85-9			
	Limit value - Eight hours		**Limit value - Short term**	
	ppm	**mg/m^3**	**ppm**	**mg/m^3**
Finland	?	0,2	?	?
	Remarks			

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 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

Information on basic physicochemical properties

Physical state	Orange-yellow crystalline solid with a characteristic odor.
Colour	Yellow orthrhombic needles from acetic acid
Odour	no data available
Melting point/freezing point	93°C
Boiling point or initial boiling point and boiling range	307.5°C at 760 mmHg
Flammability	no data available
Lower and upper explosion limit/flammability limit	no data available
Flash point	152.6°C
Auto-ignition temperature	no data available
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	0.0020339 Pa.s at 365.65 K (est)
Solubility	Soluble in benzene, ethyl ether, ethanol, chloroform, carbon disulfide
Partition coefficient n-octanol/water	log Kow = 2.18 (est)
Vapour pressure	4.05X10-4 mm Hg at 25 deg C
Density and/or relative density	1.407g/cm3
Relative vapour density	no data available
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

Chemical stability

no data available

Possibility of hazardous reactions

Moderate, when exposed to heat or flame; an oxidizer.

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 216 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

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: static; Concentration: 22.0 mg/L for 96 hr

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

AEROBIC: 3,5-Dinitrotoluene was not mineralized in water from a pond and from Waconda Bay; however, 3,5-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 5.1X10+10 mL/cell-hour, and in Waconda Bay water 0.46X10+10 mL/cell-hour(1). Mixed dinitrotoluene isomers, 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(2).

Bioaccumulative potential

An estimated BCF of 13 was calculated in fish for 3,5-dinitrotoluene(SRC), using an estimated log Kow of 2.18(1) and a regression-derived equation(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is low(SRC).

Mobility in soil

Using a structure estimation method based on molecular connectivity indices(1), the Koc of 3,5-dinitrotoluene can be estimated to be 564(SRC). Using a structure estimation method based on an estimated log Kow of 2.18(1), the Koc of 3,5-dinitrotoluene can be estimated to be 370(SRC). According to a classification scheme(2), these estimated Koc values suggest that 3,5-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: no data available

IMDG: no data available

IATA: no data available

UN Proper Shipping Name

ADR/RID: no data available

IMDG: no data available

IATA: no data available

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: III (For reference only, please check.)

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

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

Environmental hazards

ADR/RID: No

IMDG: No

IATA: No

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

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

PICCS

Not 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/