ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

4-Nitrotoluene

Revision Date:2024-03-02 Revision Number:1

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

Product identifier

Product name	: 4-Nitrotoluene
CBnumber	: CB6287780
CAS	: 99-99-0
EINECS Number	: 202-808-0
Synonyms	: 4-Nitrotoluene,1-methyl-4-nitrobenzene

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

Specific target organ toxicity – repeated exposure, Category 2

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 2

Label elements

Pictogram(s)

Signal word	Danger

Hazard statement(s)

H225 Highly Flammable liquid and vapour

H301 Toxic if swalloed

H311 Toxic in contact with skin

H319 Causes serious eye irritation

H331 Toxic if inhaled

H373 May cause damage to organs through prolonged or repeated exposure

H401 Toxic to aquatic life

H411 Toxic to aquatic life with long lasting effects

Precautionary statement(s)

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

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

P273 Avoid release to the environment.

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

P309 IF exposed or if you feel unwell:

P310 Immediately call a POISON CENTER or doctor/physician.

P311 Call a POISON CENTER or doctor/physician.

P301+P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician.

P302+P352 IF ON SKIN: wash with plenty of soap and water.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P403+P235 Store in a well-ventilated place. Keep cool.

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.

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.

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	: 4-Nitrotoluene
Synonyms	: 4-Nitrotoluene,1-methyl-4-nitrobenzene
CAS	: 99-99-0
EC number	: 202-808-0
MF	: C7H7NO2
MW	: 137.14

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

Rinse and then wash skin with water and soap. Refer for medical attention . Wear protective gloves when administering first aid.

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. Refer for medical attention .

Most important symptoms and effects, both acute and delayed

INHALATION, INGESTION, OR SKIN: Headache, flushed face, dizziness, dyspnea (difficult breathing), cyanosis, nausea, vomiting, muscular weakness, rapid pulse and respiration, irritability, and convulsions. (USCG, 1999)

Indication of any immediate medical attention and special treatment needed

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Aromatic hydrocarbons and related compounds

SECTION 5: Firefighting measures

Extinguishing media

Use dry chemical, carbon dioxide, or water spray. Water streams or foam may cause frothing. Use water spray to keep fire-exposed containers cool. Approach fire from upwind to avoid hazardous vapors and toxic decomposition products. Extinguish fire using agent suitable for surrounding fire.

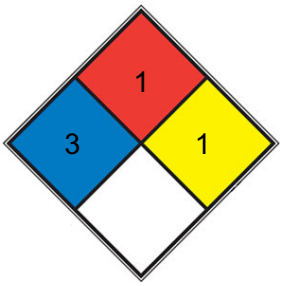
Specific Hazards Arising from the Chemical

Special Hazards of Combustion Products: Yields toxic oxides of nitrogen when burning. (USCG, 1999)

Advice for firefighters

Use water spray, powder, foam, carbon dioxide. In case of fire: keep drums, etc., cool by spraying with water.

NFPA 704



■	HEALTH	3	Short exposure could cause serious temporary or moderate residual injury (e.g. liquid hydrogen, sulfuric acid, calcium hypochlorite, hexafluorosilicic acid)
■	FIRE	1	Materials that require considerable preheating, under all ambient temperature conditions, before ignition and combustion can occur. Includes some finely divided suspended solids that do not require heating before ignition can occur. Flash point at or above 93.3 °C (200 °F). (e.g. mineral oil, ammonia)
■	REACT	1	Normally stable, but can become unstable at elevated temperatures and pressures (e.g. propene)
□	SPEC. HAZ.		

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Environmental precautions

Personal protection: chemical protection suit including self-contained breathing apparatus. Do NOT let this chemical enter the environment. Sweep spilled substance into covered containers. Carefully collect remainder. Then store and dispose of according to local regulations.

Methods and materials for containment and cleaning up

Ventilate area of spill or leak. For small quantities of liq nitrotoluene, absorb on paper towels. For small quantities of solid nitrotoluene, sweep onto paper or other suitable material. Remove to safe place (such as fume hood) & burn. Large quantities of liq nitrotoluene can be collected & atomized in suitable combustion chamber equipped with appropriate effluent gas cleaning device. Large quantities of solid nitrotoluene can be reclaimed; ... If not practical, dissolve in flammable solvent (such as alcohol) & atomize in suitable combustion chamber equipped with appropriate effluent gas cleaning device. Nitrotoluene

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. NO contact with oxidizing agents. 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 food and feedstuffs. See Chemical Dangers. Well closed.Store in a cool. dry, well-ventilated location. Separate from acids, alkalies, oxidizing materials, and reducing agents.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

TLV: 2 ppm as TWA; (skin); BEI issued.MAK: skin absorption (H); carcinogen category: 3B

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, 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

Information on basic physicochemical properties

Physical state	Crystalline Solid
Colour	Yellow
Odour	Bitter almond
Melting point/freezing point	44.5 °C. Remarks:(unstable).;51.9 °C. Remarks:(stable).
Boiling point or initial boiling point and boiling range	238.3 °C. Atm. press.:101 kPa.;53.7 °C. Atm. press.:0.13 kPa.
Flammability	Combustible Solid
Lower and upper explosion limit/flammability limit	1.6%(V)
Flash point	103 °C. Atm. press.:1 013 hPa.

Auto-ignition temperature	450 °C.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	1.2 mPa (= cP) at 60 deg C
Solubility	0.26g/l
Partition coefficient n-octanol/water	log Pow = 2.37. Temperature:25 °C.
Vapour pressure	5 mm Hg (85 °C)
Density and/or relative density	1.392
Relative vapour density	1.392
Particle characteristics	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on heating. This produces toxic fumes of nitrogen oxides. Reacts violently with strong oxidants and sulfuric acid. This generates fire and explosion hazard. Attacks some forms of plastic, rubber and coatings.

Chemical stability

Heat contributes/ ... to instability. Nitrotoluene

Possibility of hazardous reactions

Combustible when exposed to heat or flame.P-NITROTOLUENE may react violently with sodium, tetranitromethane, strong oxidizing agents , sulfuric acid and other acids. (NTP, 1992)

Conditions to avoid

no data available

Incompatible materials

Decomposes on contact with strong oxidzers; strong acids; reducing agents; strong bases; ammonia, amines producing toxic fumes, causing fire and explosion hazard. Heat above 190 deg C may cause explosive decomposition. Attacks some plastics, rubbers, and coatings.

Hazardous decomposition products

The substance decomposes on heating producing toxic fumes /of/ (nitrogen oxides).

SECTION 11: Toxicological information

Acute toxicity

- Oral: LD50 - rat (male/female) - > 2 250 mg/kg bw.
- Inhalation: LC50 - rat (male/female) - > 851 mg/m3 air.
- Dermal: LD50 - rat (male/female) - > 750 mg/kg bw.

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 nitrotoluenes. There is inadequate evidence in experimental animals for the carcinogenicity of ... 4-nitrotoluene. ... Overall evaluation: Nitrotoluenes are not classifiable as to their carcinogenicity to humans (Group 3).

Reproductive toxicity

no data available

STOT-single exposure

The substance is irritating to the eyes. 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, liver and testes.

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 - Pimephales promelas - 49.7 mg/L - 96 h.
Toxicity to daphnia and other aquatic invertebrates: EC50 - Daphnia magna - ca. 4.2 mg/L - 48 h.
Toxicity to algae: EC50 - Chlorella pyrenoidosa - 22 mg/L - 96 h.
Toxicity to microorganisms: EC50 - other fungi: Phytium ultimum Trow. - ca. 30 mg/L - 88 h.

Persistence and degradability

AEROBIC: 4-Nitrotoluene, present at 100 mg/L, reached 0.8% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese MITI test(1) which indicates the compound is not readily biodegradable(1). Two studies demonstrated that 4-nitrotoluene could be completely degraded by unacclimated sludge withing two weeks when lower concentrations of 4-nitrotoluene (10 ppm) were used(2,3). When nitrotoluene-adapted activated sludges were used as an inoculum, however, 4-nitrotoluene was almost completely degraded (~98%) within 5 days, even when higher concentrations (200 mg/L) of 4-nitrotoluene were used(4). 2-Amino-4-methylphenol has been identified as a microbial degradation product of 4-nitrotoluene(5). Using a mixed culture isolated from a contaminated soil (near an ammunition

plant), 4-nitrotoluene (at initial concentrations of 5 mg/L) degraded completely in 1 to 3 days in aerobic batch and continuous reactor tests(6).

Bioaccumulative potential

An estimated BCF of 13 was calculated for 4-nitrotoluene(SRC), using a log Kow of 2.37(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). The BCF for 4-nitrotoluene has been measured to be low in an unidentified fish and in carp (Carprinus carpio)(4,5).

Mobility in soil

A log Koc value of 2.14 (Koc = 138) was experimentally determined for 4-nitrotoluene in a single lake sediment from China(1). Using a structure estimation method based on molecular connectivity indices(2), the Koc of 4-nitrotoluene can be estimated to be 363(SRC). According to a classification scheme(3), the estimated and experimental Koc values suggest that 4-nitrotoluene is expected to have high to moderate 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: UN3446 (For reference only, please check.)

IMDG: UN3446 (For reference only, please check.)

IATA: UN3446 (For reference only, please check.)

UN Proper Shipping Name

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

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

IATA: NITROTOLUENES, 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

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

Specific treatment is necessary in case of poisoning with this substance; the appropriate means with instructions must be available.Depending on the degree of exposure, periodic medical examination is suggested.