

## Chemical Safety Data Sheet MSDS / SDS

## 4-Nitrotoluene

Revision Date:2025-04-05 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,p-Nitrotoluene

## 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 swallowed  
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

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## SECTION 3: Composition/information on ingredients

### Substance

Product name	: 4-Nitrotoluene
Synonyms	: 4-nitrotoluene,p-Nitrotoluene
CAS	: 99-99-0
EC number	: 202-808-0
MF	: C7H7NO2
MW	: 137.14

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## 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

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## 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.

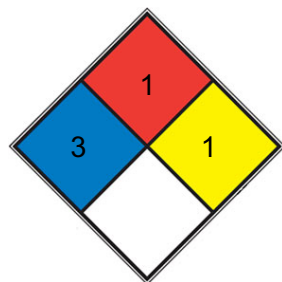
### Specific Hazards Arising from the Chemical

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.

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## 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

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## 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.

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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

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## 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 oxidizers; 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).

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## 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.

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## **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 within 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

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## 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.

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## 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

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## **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.

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## **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](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.

### 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.