Chemical Safety Data Sheet MSDS / SDS

3-nitrotoluene SDS

Revision Date:2024-04-25 Revision Number:1

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

Product identifier

Product name: 3-nitrotoluene

CAS: 99-08-1

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.in

Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090

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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

GHS label elements, including precautionary statements

Pictogram(s)

Signal word Danger

Hazard statement(s)

H301 Toxic if swallowed
H311 Toxic in contact with skin
H331 Toxic if inhaled
H373 May cause damage to organs through prolonged or repeated exposure

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

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.

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 which do not result in classification

no data available

SECTION 3: Composition/information on ingredients

Substance

Chemical name:	3-nitrotoluene
Common names and synonyms:	3-nitrotoluene
CAS number:	99-08-1
EC number:	202-728-6
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Fresh air, rest. Refer for medical attention.

Following skin contact

Remove contaminated clothes. Rinse and then wash skin with water and soap.

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/effects, acute and delayed

INHALATION, INGESTION OR SKIN ABSORPTION: Headache, flushing of face, dizziness, difficult breathing, cyanosis, nausea, vomiting, muscular weakness, increased pulse and respiratory rate, irritability and convulsions. EYES: Slight irrita- tion. SKIN: Slight irritation. (USCG, 1999)

Indication of immediate medical attention and special treatment needed, if necessary

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

Suitable extinguishing media

To fight fire use water, carbon dioxide, dry chemical.

Specific hazards arising from the chemical

Special Hazards of Combustion Products: Emits toxic fumes of oxides of nitrogen. Behavior in Fire: Emits toxic fumes. (USCG, 1999)

Special protective actions for fire-fighters

Use water spray, powder, foam, carbon dioxide. Combat fire from a sheltered position.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Ventilation. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. Then store and dispose of according to local regulations.

Environmental precautions

Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus. Ventilation. Collect leaking liquid in covered containers. Absorb remaining liquid in sand or inert absorbent. 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 liquid nitrotoluene, absorb on paper towels. For small quantities of solid nitrotoluene, sweep onto paper or other suitable material. Remove to a safe place (such as a fume hood) and burn paper. Large quantities of liquid nitrotoluene can be collected and atomized in a suitable combustion chamber equipped with an appropriate effluent gas cleaning device. Large quantities of solid nitrotoluene can be reclaimed; however, if this is not practical, dissolve in a flammable solvent (such as alcohol) and atomize in a suitable combustion chamber equipped with an appropriate effluent gas cleaning device. nitrotoluene

SECTION 7: Handling and storage

Precautions for safe handling

NO open flames. NO contact with strong oxidizing agents or sulfuric acid. 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 strong oxidants, sulfuric acid and food and feedstuffs. Cool. Dry. Keep in a well-ventilated room.Separated from strong oxidants, sulfuric acid, food and feedstuffs. Cool. Dry. Keep in a well-ventilated room.

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

Appropriate engineering 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, such as personal protective equipment (PPE)

Eye/face protection

Wear face shield or eye protection in combination with breathing protection.

Skin protection

Protective gloves. Protective clothing.

Respiratory protection

Use ventilation, local exhaust or breathing protection.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Liquid.
Colour:	Clear yellow.
Odour:	Weak, aromatic odor
Melting point/freezing point:	16.1 °C.
Boiling point or initial boiling point and boiling range:	231.9 °C. Atm. press.:101.3 kPa.;156.9 °C. Atm. press.:13.3 kPa.;50.2 °C. Atm. press.:0.13 kPa.
Flammability:	Class IIIB Combustible Liquid: Fl.P. at or above 200°F.
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	106 °C. Atm. press.:1 013 mBar.

Auto-ignition temperature:	450 °C.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	dynamic viscosity (in mPa s) = 2.33. Temperature:20°C.
Solubility:	Insoluble in water
Partition coefficient n-octanol/water:	log Pow = 2.4.
Vapour pressure:	16 Pa. Temperature:20 °C. Remarks:=0.16 hPa= 0.016 kPa.
Density and/or relative density:	1.16. Temperature:20 °C.
Relative vapour density:	4.73 (vs air)
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

Decomposes on burning. This produces toxic gases including carbon monoxide and nitrogen oxides. Reacts with strong oxidants and sulfuric acid. This generates fire and explosion hazard. Attacks plastics, rubber and coatings.

Chemical stability

Heat contributes/ ... to instability. Nitrotoluene

Possibility of hazardous reactions

Combustible when exposed to heat, flame or oxidizers.M-NITROTOLUENE reacts with sulfuric acid, strong oxidizing agents and reducing agents.

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 burning producing toxic gases, including carbon monoxide and nitrogen oxides.

SECTION 11: Toxicological information

Acute toxicity

Oral: LD50 - rat (male) - 2 121 mg/kg bw.

Inhalation: LC50 - rat (male/female) - > 880 mg/m3 air.

Dermal: LD50 - rat - > 1 157 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 3-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 mildly irritating to the eyes and skin. The substance may cause effects on the blood. This may result in the formation of methaemoglobin. Medical observation is indicated. The effects may be delayed.

STOT-repeated exposure

no data available

Aspiration hazard

A harmful contamination of the air will be reached rather slowly on evaporation of this substance at 20°C.

SECTION 12: Ecological information

Toxicity

Toxicity to fish: LC50 - Pimephales promelas - 30 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: LC50 - Daphnia magna - 7.5 mg/L - 48 h.

Toxicity to algae: EC50 - Chlorella pyrenoidosa - 14 mg/L - 96 h.

Toxicity to microorganisms: EC50 - Tetrahymena pyriformis - 50 mg/L - 24 h.

Persistence and degradability

AEROBIC: 3-Nitrotoluene, present at 100 mg/L, reached 2% of its theoretical BOD in 2 weeks using an activated sludge inoculum at 30 mg/L in the Japanese Ministry of Industry and Trade (MITI) test, which employs a mixed inoculum obtained from freshwater, soil, and sludge(1). Using unacclimated sludge as the inoculum(2) but lower concentrations of 3-nitrotoluene (10 ppm), complete degradation was observed to occur within 14 days. Other evidence supports complete aerobic degradation of 10 mg/L 3-nitrotoluene within 2 weeks when incubated in adapted aerobic composite river sediment and sewage sludges(3). When nitrotoluene-adapted activated sludges were used as an inoculum, however, 3-nitrotoluene (200 mg/L) was almost completely

degraded (i.e. 98% removal) within 5 days when incubated at 20 deg C(4). Using a mixed culture isolated from a contaminated soil (near an ammunition plant), 3-nitrotoluene (at initial concentrations of 5 and 12 mg/L) degraded completely in 4 days in aerobic batch and continuous reactor tests(5).

Bioaccumulative potential

The BCF for 3-nitrotoluene in fish (Poecilia reticulata) was been experimentally determined to be 16(1). The BCF in carp (Cyprinus carpio) ranged from 0.47 to 12 at test concentrations of 2.5-25 ppb 3-nitrotoluene over a 6-week exposure period(2). According to a classification scheme(2), these BCF values suggest 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-nitrotoluene can be estimated to be 363(SRC). According to a classification scheme(2), this estimated Koc value suggests that 3-nitrotoluene is expected to have moderate mobility in soil. Field monitoring at a munition factory site in Melbourne Australia found that 3-nitrotoluene migrated large distances in the subsurface soils(3); 3-nitrotoluene is reported to have low soil Kd sorption coefficients in a variety of soils types(3) indicating it will leach.

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: UN1664 (For reference only, please check.)
IMDG: UN1664 (For reference only, please check.)
IATA: UN1664 (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: NITROTOLUENES, LIQUID (For reference only, please check.)
IMDG: NITROTOLUENES, LIQUID (For reference only, please check.)
IATA: NITROTOLUENES, LIQUID (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: 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

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

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.