

# SAFETY DATA SHEETS

According to the UN GHS revision 10

## 1: Identification

### 1.1 GHS Product identifier

Product name 3-Nitrotoluene

### 1.2 Other means of identification

Product number 99-08-1

Other names 3-Nitrotoluene

### 1.3 Recommended use of the chemical and restrictions on use

Identified uses Industrial and scientific research use.

Uses advised against no data available

### 1.4 Supplier's details

Company MolBest.com

Address MolBest.com

Telephone MolBest.com

### 1.5 Emergency phone number

Emergency phone number MolBest.com

Service hours MolBest.com

## 2: Hazard identification

### 2.1 Emergency Overview

Highly toxic substances, even small amounts of which can cause death or serious health effects. They can enter the body through inhalation, skin contact, or ingestion. Immediate protective measures must be taken to avoid any contact.

### 2.2 GHS Classification

Acute toxicity, oral; acute toxicity, dermal; acute toxicity, inhalation : Category 3

Acute toxicity, oral : Category 3

Acute toxicity, dermal : Category 3

Acute toxicity, inhalation : Category 3

Specific target organ toxicity, repeated exposure : Category 2

Hazardous to the aquatic environment, long-term hazard : Category 2

### 2.3 GHS label elements, including precautionary statements

**Pictogram(s)****Signal word**

Danger

**Hazard statement(s)**

H301+H311+H331 Toxic if swallowed, in contact with skin or if inhaled  
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  
H411 Toxic to aquatic life with long lasting effects

**Precautionary statement(s)****Prevention**

P260 Do not breathe dust/fume/gas/mist/vapors/spray.  
P261 Avoid breathing dust/fume/gas/mist/vapors/spray.  
P262 Do not get in eyes, on skin, or on clothing.  
P264 Wash hands [and ...] thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P271 Use only outdoors or in a well-ventilated area.  
P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...

**Response**

P316 Get emergency medical help immediately.  
P319 Get medical help if you feel unwell.  
P321 Specific treatment (see ... on this label).  
P330 Rinse mouth.  
P391 Collect spillage.  
P301+P316 IF SWALLOWED, Get emergency medical help immediately.  
P302+P352 IF ON SKIN, wash with plenty of water/...  
P304+P340 IF INHALED, Remove person to fresh air and keep comfortable for breathing.  
P361+P364 Take off immediately all contaminated clothing and wash it before reuse.

**Storage**

P405 Store locked up.  
P403+P233 Store in a well-ventilated place. Keep container tightly closed.

**Disposal**

P501 Dispose of contents/container to ...

## 2.4 Physical and chemical

Some substances may also be flammable or corrosive. Mixing with other substances may produce toxic products. Highly volatile substances can form toxic vapor clouds, expanding the hazard range.

## 2.5 Health hazards

Acute toxicity, May cause respiratory failure, cardiac arrest, nervous system depression, or organ failure. Severe symptoms may appear within a short period of exposure (minutes to hours). Long-term effects may include permanent organ damage.

## 2.6 Environmental hazards

It is extremely toxic to aquatic organisms and terrestrial ecosystems, and even a small release can cause large-scale biological mortality. It may persist in the environment and accumulate through the food chain, causing long-term damage to ecosystems.

## 2.7 Other hazards which do not result in classification

no data available

## 3: Composition/information on ingredients

### 3.1 Substances

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

## 4: First-aid measures

### 4.1 General advice

Stop contact immediately and move to a safe area; bring the material SDS document and call emergency services immediately; record the route of exposure (inhalation/skin/ingestion), exposure time and dosage for the doctor's judgment.

### 4.2 If inhaled

Quickly transfer the patient to a place with fresh air, keep the patient lying flat with the head tilted to one side (to prevent suffocation by vomitus); if cyanosis or breathing difficulties occur, immediately give oxygen (flow rate 5-10L/min); it is strictly forbidden to feed/drink water to the unconscious person, and seek medical attention immediately.

### 4.3 In case of skin contact

Immediately remove contaminated clothing (if clothing is stuck to the skin, cut it with scissors to avoid tearing it). Rinse the affected area with plenty of running water for 20-30 minutes (the water temperature should be around 37°C, avoiding excessive heat or cold). If the skin is damaged, cover it with sterile gauze after rinsing. Do not apply ointment.

### 4.4 In case of eye contact

Immediately flush with an eyewash station for 15 minutes (open the eyelids to ensure thorough flushing of the upper and lower fornixes); wear a light-shielding eye mask after flushing to avoid strong light stimulation, and immediately seek medical attention from an ophthalmologist (bring along the substance SDS).

### 4.5 If swallowed

Self-induced vomiting is strictly prohibited (especially with corrosive and toxic substances, which may cause secondary burns to the esophagus). If the patient is conscious and not convulsing, they can drink 50-100ml of milk under the guidance of a doctor (to protect the gastric mucosa).

### 4.6 Most important symptoms and effects, both acute and delayed

Acute symptoms: nausea and vomiting, abdominal pain, dyspnea, convulsions, confusion, and decreased blood pressure; delayed symptoms: liver and kidney damage (appearing within 24-72 hours), methemoglobinemia (such as nitrite poisoning).

#### **4.7 Protection of first-aiders**

Rescuers must wear fully enclosed chemical protective clothing, a gas mask (with a targeted gas filter cartridge, such as for organic vapors and acid gases), and chemical protective gloves; avoid direct contact with the patient's vomitus/secretions, and wash hands immediately with chlorine-containing disinfectant after contact.

#### **4.8 Notes to physician**

Inform the physician of the substance's toxicity (e.g., oral LD50 = 5 mg/kg) and route of exposure; prioritize gastric lavage (physician evaluation required for appropriateness) and administer antidotes (e.g., atropine for organophosphate poisoning); monitor liver and kidney function, electrolytes, and coagulation function.

### **5: Fire-fighting measures**

#### **5.1 Unsuitable extinguishing media**

It is strictly forbidden to use fire extinguishing agents that may cause the spread of toxic substances (such as high-pressure water jets); if flammable liquids are involved, avoid using carbon dioxide (which may cause toxic vapor condensation).

#### **5.2 Specific hazards during fire fighting**

Combustion may be accompanied by the release of highly toxic substances (such as cyanide and arsenide), which are fatal by inhalation or skin contact; the combustion of flammable components can easily cause explosions and intensify the spread of toxic substances; toxic vapors are heavier than air and tend to accumulate in low-lying areas.

#### **5.3 Hazardous combustion products**

Highly toxic gases (such as hydrogen chloride, hydrogen fluoride, phosgene), carbon monoxide, nitrogen oxides; some contain heavy metal components that release toxic fumes such as mercury and lead.

#### **5.4 Specific extinguishing methods**

For small areas: use dry powder fire extinguishing agent to extinguish the fire, and dilute the toxic vapor with mist water (avoid direct spraying); for large areas: give priority to evacuation. If fire extinguishing is necessary, set up a fire extinguishing point upwind and cover it with foam (to isolate oxygen); after extinguishing the fire, test the area for toxicity concentration (entry is allowed only when the value is below MAC).

#### **5.5 Special protective equipment for fire-fighters**

Wear fully enclosed chemical protective clothing, gas masks (with targeted gas filter boxes, such as organic vapor + acidic gas), and chemical protective gloves (made of fluororubber); carry a portable toxic gas detector; equipment must be disinfected after the operation, and personnel must undergo health monitoring.

## 6: Accidental release measures

### 6.1 Protective measures for workers

Wear fully enclosed chemical protective clothing, positive pressure air respirator, chemical protective gloves (toxic-resistant type) and goggles; avoid direct contact with the skin and wash immediately after work.

### 6.2 Environmental protection measure

Isolate the 30-meter contaminated area to prevent the leak from spreading through rainwater/groundwater; take samples of water/soil for testing, and use activated carbon adsorption (organic poison) or neutralizer (inorganic poison) for treatment when exceeding the standard; strictly prohibit the leak from entering the drinking water source.

### 6.3 Containment methods for leaked chemicals

Collect liquids in corrosion-resistant sealed containers (marked with "toxic substances"); collect solids in chemical-resistant bags (to avoid dust); and store them separately in a hazardous waste warehouse after collection, away from food/feed.

### 6.4 Cleanup methods for chemical spills

Small leakage: absorb with special absorbent cotton (toxic-resistant) and put into chemical-proof bag; large leakage: professionals use chemical-proof pump to transfer to special storage tank; after cleaning, treat the ground with neutralizer (weak base for acid poison and weak acid for alkali poison).

### 6.5 Measures to prevent the spread of leaks

Set up a 30-meter isolation zone and prohibit unauthorized personnel from entering; volatile toxic substances require explosion-proof ventilation to reduce gas concentration; use chemical defense isolation belts to block them, and focus on monitoring low-lying areas (to prevent the accumulation of toxic substances).

### 6.6 Container leakage treatment

Minor leaks: Seal with compatible sealant; Serious leaks: Evacuate immediately, close the upstream valve (if safe), and have the toxic material disposal team handle it. It is strictly forbidden to open the container without authorization.

### 6.7 Special considerations

Workers must receive poisoning first aid training and carry antidotes (if applicable). In case of skin contact, flush immediately with plenty of water for 15 minutes. In case of inhalation poisoning, move immediately to fresh air and seek medical attention.

## 7: Handling and storage

### 7.1 Safe storage conditions

Store in a closed, impermeable dedicated warehouse (the walls are made of anti-corrosion materials, such as polyethylene coating); the container is made of corrosion-resistant material (such as

polytetrafluoroethylene, glass-lined steel), with a double sealing cover (threaded cover + nitrile rubber sealing ring); the warehouse is equipped with a negative pressure ventilation system (air changes ? 8 times/hour), and the exhaust gas must be treated with activated carbon adsorption (adsorption efficiency ? 95%).

## 7.2 Storage precautions

Store them separately from food, feed, and medicine (isolation distance ? 3 meters), and strictly prohibit them from being adjacent to drinking water sources; clearly mark "highly toxic" and H code on container labels and store them separately on locked shelves; check the sealing of containers weekly and immediately transfer them to the emergency treatment area if any leakage is found; workers must wear fully enclosed chemical protective clothing before entering the warehouse.

## 7.3 VCI Storage Grade

Level 1 (highest): The inner wall of the metal container is coated with a VCI anti-rust coating (thickness ? 50?m), and the outer surface of the container is wrapped with a vapor phase anti-rust film; the concentration of toxic substances in the warehouse is tested monthly to ensure that it is lower than the MAC value (for example, MAC of oral toxic substances ? 0.1mg/m<sup>3</sup>).

## 7.4 Recommended storage temperature

10-30?, avoid extreme temperatures (below 0? or above 35?); volatile toxic substances must be kept at a temperature ?25? to reduce vapor release; refrigerated storage substances (such as certain biotoxins) must be maintained at 2-8? and equipped with dual power supply protection (if the label has a recommended storage temperature, the label shall prevail).

## 7.5 Handling

For precautions see Safety Data Sheet section 2

Advice on safe handling : Work under hood. Do not inhale substance/mixture.

# 8: Exposure controls/personal protection

## 8.1 Respiratory protection

Choose according to the exposure route: volatile substances require positive pressure air respirators; dust/aerosols require powered air-purifying respirators to ensure the protection factor (APF) ? 1000.

## 8.2 Recommended Filter type

For organic toxic substances, choose Type A filter cartridge (to protect against organic vapors, such as benzene and methanol); for inorganic toxic substances, choose Type B (to protect against ammonia) or Type E (to protect against acidic gases, such as hydrogen chloride); for dust, add Type P3 filter cotton.

## 8.3 Eye/face protection

Wear a full-face chemical protective mask. The mask material must be resistant to toxic penetration (such as fluororubber), and the lens must be anti-fog and anti-chemical corrosion.

## 8.4 Skin and body protection

Wear fully enclosed chemical protective clothing. The material must be compatible with toxic substances (such as polyethylene + neoprene composite material); the cuffs and ankles must be tightened and

equipped with emergency escape zippers.

## 8.5 Hand protection

Wear toxic and chemical-resistant gloves, preferably made of fluororubber or butyl rubber, with a length of 30 cm, covering the forearm, and change every 4 hours

## 8.6 Hygiene measures

Immediately after the operation, clean the skin with a special detergent (such as a weak alkaline detergent), and then rinse with running water for 15 minutes; clothes need to be disinfected at high temperature (above 60°C) before washing; regular physical examinations (blood routine, liver and kidney function tests every 3 months).

# 9: Physical and chemical properties and safety characteristics

<b>Physical state</b>	yellow-green liquid
<b>Colour</b>	Yellow liquid [Note: A solid below 59 degrees F]
<b>Odour</b>	Weak, aromatic odor
<b>Melting point/freezing point</b>	139°C(lit.)
<b>Boiling point or initial boiling point and boiling range</b>	232°C
<b>Flammability</b>	Class IIIB Combustible Liquid: Fl.P. at or above 93.33°C.Combustible. Gives off irritating or toxic fumes (or gases) in a fire.
<b>Lower and upper explosion limit/flammability limit</b>	2.2%(V)
<b>Flash point</b>	106°C(lit.)
<b>Auto-ignition temperature</b>	no data available
<b>Decomposition temperature</b>	The substance decomposes on burning producing toxic gases, including carbon monoxide and nitrogen oxides.
<b>pH</b>	no data available
<b>Kinematic viscosity</b>	2.33 cP at 20°C
<b>Solubility</b>	In water:insoluble
<b>Partition coefficient n-octanol/water</b>	log Kow = 2.45
<b>Vapour pressure</b>	1 mm Hg ( 50.2 °C)
<b>Density and/or relative density</b>	1.157

<b>Relative vapour density</b>	4.73 (vs air)
<b>Particle characteristics</b>	no data available

## 10: Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

/Heat contributes/ ... to instability. /Nitrotoluene/

### 10.3 Possibility of hazardous reactions

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

### 10.4 Conditions to avoid

no data available

### 10.5 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°C may cause explosive decomposition. Attacks some plastics, rubbers, and coatings.

### 10.6 Hazardous decomposition products

The substance decomposes on burning producing toxic gases, including carbon monoxide and nitrogen oxides.

## 11: Toxicological information

### 11.1 Acute toxicity

Oral: LD50 Mouse oral 1231 mg/kg bw  
Inhalation: LC50 Rat inhalation >2.417 mg/L /1 hr  
Dermal: no data available

### 11.2 Skin corrosion/irritation

no data available

### 11.3 Serious eye damage/irritation

no data available

## 11.4 Respiratory or skin sensitization

no data available

## 11.5 Germ cell mutagenicity

no data available

## 11.6 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).

## 11.7 Reproductive toxicity

no data available

## 11.8 STOT-single exposure

no data available

## 11.9 STOT-repeated exposure

no data available

## 11.10 Aspiration hazard

no data available

# 12: Ecological information

## 12.1 Toxicity

Toxicity to fish: LC50; Species: Brachydanio rerio (Zebra Danio); Conditions: freshwater, flow through, 23°C, pH 8.15; Concentration: 33100 ug/L for 48 hr /formulation

Toxicity to daphnia and other aquatic invertebrates: EC50; Species: Daphnia magna (Water Flea); Conditions: freshwater, static; Concentration: 7400 ug/L for 48 hr; Effect: intoxication, immobilization />99.5% purity formulation

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

## 12.2 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°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).

### 12.3 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).

### 12.4 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.

### 12.5 Other adverse effects

no data available

## 13: Disposal considerations

### 13.1 Disposal methods for waste chemicals

This must be handled by a qualified unit that handles highly toxic waste, using high-temperature incineration (800-1000°C) or chemical neutralization (such as oxidative decomposition) to completely destroy the toxicity. Liquid highly toxic substances must be solidified before incineration. Those that cannot be incinerated must be stabilized/solidified before being safely landfilled.

### 13.2 Precautions

Disposal personnel must wear fully enclosed chemical protective suits and positive pressure respirators; waste must be strictly classified and packaged to prevent leakage; exhaust gas and wastewater generated during the disposal process must meet discharge standards; mixing with other types of waste is prohibited; and disposal records must be kept for at least 10 years for traceability.

## 14: Transport information

### 14.1 UN Number

ADR/RID: UN1664

IMDG: UN1664

IATA: UN1664

### 14.2 UN Proper Shipping Name

ADR/RID: NITROTOLUENES,  
LIQUID

IMDG: NITROTOLUENES,  
LIQUID

IATA: NITROTOLUENES,  
LIQUID

### 14.3 Transport hazard class(es)

ADR/RID: 6.1

IMDG: 6.1

IATA: 6.1

### 14.4 Packing group, if applicable

ADR/RID: II

IMDG: II

IATA: II

### 14.5 Environmental hazards

ADR/RID: no

IMDG: no

IATA: no

### 14.6 Special precautions for user

no data available

### 14.7 Transport in bulk according to IMO instruments

no data available

## 15: Regulatory information

### 15.1 Safety, health and environmental regulations specific for the product in question

Chemical name	Common names and synonyms	CAS number	EC number
3-Nitrotoluene	3-Nitrotoluene	99-08-1	202-728-6
New Zealand Inventory of Chemicals (NZIoC)			Listed.
Philippines Inventory of Chemicals and Chemical Substances (PICCS)			Listed.
Vietnam National Chemical Inventory			Not Listed.
Australian Inventory of Industrial Chemicals (AIIC)			Not Listed.
Catalogue of Strictly Restricted Toxic Chemicals in China			Not Listed.
China Catalog of Hazardous chemicals 2015			Listed.
European INventory of Existing Commercial chemical Substances			Not Listed.
IARC Monographs on the Evaluation of Carcinogenic Risks to Humans			Listed.
TSCA Inventory of Chemical Substances			Listed.

## 16: Other information

#### Information on revision

SDS Creation Date July 1, 2025

SDS Revision Date July 1, 2025

#### Abbreviations and acronyms in SDS

- 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%

### SDS 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/>

**Any questions regarding this Safety Data Sheet, Please send your inquiry to [info@MolBest.com](mailto:info@MolBest.com)**

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