

Chemical Safety Data Sheet MSDS / SDS

3-Nitrotoluene

Revision Date:2024-12-21 Revision Number:1

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

Product identifier

Product name : 3-Nitrotoluene
CBnumber : CB7854761
CAS : 99-08-1
EINECS Number : 202-728-6
Synonyms : MXD6,3-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

GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Danger

Precautionary statements

P501 Dispose of contents/container to....

P405 Store locked up.

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

P391 Collect spillage. Hazardous to the aquatic environment

P311 Call a POISON CENTER or doctor/physician.

P310 Immediately call a POISON CENTER or doctor/physician.

P309 IF exposed or if you feel unwell:

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

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

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

P284 Wear respiratory protection.

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

P273 Avoid release to the environment.

P271 Use only outdoors or in a well-ventilated area.

P270 Do not eat, drink or smoke when using this product.

P264 Wash skin thoroughly after handling.

P264 Wash hands thoroughly after handling.

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

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

P202 Do not handle until all safety precautions have been read and understood.

P201 Obtain special instructions before use.

Hazard statements

H411 Toxic to aquatic life with long lasting effects

H401 Toxic to aquatic life

H373 May cause damage to organs through prolonged or repeated exposure

H371 May cause damage to organs

H361 Suspected of damaging fertility or the unborn child

H332 Harmful if inhaled

H331 Toxic if inhaled

H330 Fatal if inhaled

H320 Causes eye irritation

H319 Causes serious eye irritation

H311 Toxic in contact with skin

H302 Harmful if swallowed

H301 Toxic if swallowed

SECTION 3: Composition/information on ingredients

Substance

Product name	: 3-Nitrotoluene
Synonyms	: MXD6,3-nitrotoluene
CAS	: 99-08-1
EC number	: 202-728-6
MF	: C7H7NO2
MW	: 137.14

SECTION 4: First aid measures

Description of first aid measures

General advice

Consult a physician. Show this material safety data sheet to the doctor in attendance.

If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

In case of skin contact

Wash off with soap and plenty of water. Consult a physician.

In case of eye contact

Flush eyes with water as a precaution.

If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

Most important symptoms and effects, both acute and delayed

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

Indication of any immediate medical attention and special treatment needed

No data available

SECTION 5: Firefighting measures

Extinguishing media**Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

Special hazards arising from the substance or mixture

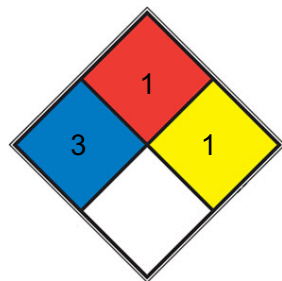
Carbon oxides, Nitrogen oxides (NO_x)

Advice for firefighters

Wear self-contained breathing apparatus for firefighting if necessary.

Further information

No data available

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

Use personal protective equipment. Avoid breathing vapors, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas.
For personal protection see section 8.

Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Methods and materials for containment and cleaning up

Soak up with inert absorbent material and dispose of as hazardous waste. Keep in suitable, closed containers for disposal.

Reference to other sections

For disposal see section 13.

SECTION 7: Handling and storage

Precautions for safe handling

Avoid contact with skin and eyes. Avoid inhalation of vapor or mist. For precautions see section 2.2.

Conditions for safe storage, including any incompatibilities

Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage. Store in cool place.

Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

SECTION 8: Exposure controls/personal protection

control parameter

Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

Exposure controls

Appropriate engineering controls

Handle in accordance with good industrial hygiene and safety practice. Wash hands before breaks and at the end of workday.

Personal protective equipment

Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of Regulation (EU) 2016/425 and the standard EN 374 derived from it.

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,3 mm Break through time: 480 min

Material tested:Butoject? (KCL 897 / Aldrich Z677647, Size M)

Splash contact Material: Nitrile rubber

Minimum layer thickness: 0,4 mm Break through time: 30 min

Material tested:Camatril? (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the EC approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

Body Protection

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

Respiratory protection

Where risk assessment shows air-purifying respirators are appropriate use a full- face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

Control of environmental exposure

Prevent further leakage or spillage if safe to do so. Do not let product enter drains. Discharge into the environment must be avoided.

Exposure limits

NIOSH REL: TWA 2 ppm (11 mg/m³), IDLH 200 ppm; OSHA PEL: TWA 5 ppm (30 mg/m³); ACGIH TLV: TWA 2 ppm (adopted).

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance	yellow liquid
Odour	characteristic
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point/range: 14 - 16 °C - lit.
Initial boiling point and boiling range	230 - 231 °C - lit.
Flash point	215 °F
Evaporation rate	No data available

Flammability (solid, gas)	No data available
Upper/lower flammability or explosive limits	2.2%(V)
Vapour pressure	1 mm Hg (50.2 °C)
Vapour density	4.73 (vs air)
Relative density	1,157 g/cm ³ at 25 °C
Water solubility	0,419 g/l at 20 °C
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	270 °C -
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available
Henry's Law Constant	9.31 at 25 °C (thermodynamic method-GC/UV spectrophotometry, Altschuh et al., 1999)

Other safety information

No data available

SECTION 10: Stability and reactivity

Reactivity

No data available

Chemical stability

Stable under recommended storage conditions.

Possibility of hazardous reactions

No data available

Conditions to avoid

No data available

Incompatible materials

No data available

Hazardous decomposition products

Hazardous decomposition products formed under fire conditions. - Carbon oxides, Nitrogen oxides (NO_x)

Other decomposition products - No data available In the event of fire: see section 5

SECTION 11: Toxicological information

Information on toxicological effects

Acute toxicity

LD50 Oral - Rat - male and female - 1.784 mg/kg (OECD Test Guideline 401)

Skin corrosion/irritation

Skin - Rabbit

Result: No skin irritation - 4 h (OECD Test Guideline 404)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: No eye irritation - 24 h (OECD Test Guideline 405)

Respiratory or skin sensitization Germ cell mutagenicity

Mutagenicity (mammal cell test): chromosome aberration.

Chinese hamster ovary cells Result: negative

Ames test

Salmonella typhimurium Result: negative

Rat - male - Liver cells Result: negative (ECHA)

Carcinogenicity

IARC: No ingredient of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

Reproductive toxicity

Specific target organ toxicity - single exposure Specific target organ toxicity - repeated exposure

May cause damage to organs through prolonged or repeated exposure.

Aspiration hazard Additional Information

RTECS: XT2975000

Absorption into the body leads to the formation of methemoglobin which in sufficient concentration causes cyanosis. Onset may be delayed 2 to 4 hours or longer.

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Toxicity

Acute oral LD50 for guinea pigs 3,600 mg/kg, mice 330 mg/kg, rats 1,072 mg/kg, rabbits 2,400 (quoted, RTECS, 1985).

SECTION 12: Ecological information

Toxicity

Toxicity to fish

flow-through test LC50 - Danio rerio (zebra fish) - 35,3 mg/l - 96 h (OECD Test Guideline 203)

Toxicity to daphnia and other aquatic invertebrates

static test EC50 - Daphnia magna (Water flea) - 7,4 mg/l - 48 h Remarks: (ECHA)

Toxicity to algae

Growth inhibition ErC50 - Chlorella pyrenoidosa - 14 mg/l - 96 h (OECD Test Guideline 201)

Toxicity to bacteria

EC50 - Photobacterium phosphoreum - 3,95 mg/l - 15 min Remarks: (IUCLID)

Persistence and degradability

Biodegradability aerobic - Exposure time 14 d

Result: 2 % - Not readily biodegradable. (OECD Test Guideline 301C)

Bioaccumulative potential

Mobility in soil

Results of PBT and vPvB assessment

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

Other adverse effects

SECTION 13: Disposal considerations

Waste treatment methods

Product

Offer surplus and non-recyclable solutions to a licensed disposal company. Waste material must be disposed of in accordance with the Directive on waste 2008/98/EC as well as other national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

Incompatibilities

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

Waste Disposal

Controlled incineration-care must be taken to maintain complete combustion at all times. Incineration of large quantities may require scrubbers to control the emission of nitrogen oxides.

Contaminated packaging

Dispose of as unused product.

SECTION 14: Transport information

UN number

ADR/RID: 1664 IMDG: 1664 IATA: 1664

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	Packaging group	
	ADR/RID: II IMDG: II	IATA: II
14.5	Environmental hazards	
	ADR/RID: yes IMDG Marine pollutant: yes	IATA: no

SECTION 15: Regulatory information

Safety, health and environmental regulations/legislation specific for the substance or mixture

Regulations on the Safety Management of Hazardous Chemicals

China Catalog of Hazardous chemicals 2015: Listed. website: <https://www.mem.gov.cn/>

Measures for Environmental Management of New Chemical Substances

Vietnam National Chemical Inventory: Listed. website: <https://chemicaldata.gov.vn/>

United States Toxic Substances Control Act (TSCA) Inventory: Listed. website: <https://www.epa.gov/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS): Listed. website: <https://emb.gov.ph/>

New Zealand Inventory of Chemicals (NZIoC): Listed. website: <https://www.epa.govt.nz/>

Korea Existing Chemicals List (KECL): Listed. website: <http://ncis.nier.go.kr>

European Inventory of Existing Commercial Chemical Substances (EINECS): Listed. website: <https://echa.europa.eu/>

EC Inventory: Listed.

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC): Listed. website: <https://www.mee.gov.cn/>

SECTION 16: Other information

Abbreviations and acronyms

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

STEL: Short term exposure limit

TWA: Time Weighted Average

References

【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:

http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en

【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>

【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

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.

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.