

Chemical Safety Data Sheet MSDS / SDS

N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine SDS

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

Section 1	Section 2	Section 3	Section 4	Section 5	Section 6	Section 7	Section 8
Section 9	Section 10	Section 11	Section 12	Section 13	Section 14	Section 15	Section 16

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

Product name: N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine

CAS: 40487-42-1

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

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SECTION 2: Hazards identification**Classification of the substance or mixture**

Skin sensitization, Category 1

Hazardous to the aquatic environment, short-term (Acute) - Category Acute 1

Hazardous to the aquatic environment, long-term (Chronic) - Category Chronic 1

GHS label elements, including precautionary statements

Pictogram(s)



Signal word

Warning

Hazard statement(s)

H317 May cause an allergic skin reaction

H410 Very toxic to aquatic life with long lasting effects

Precautionary statement(s)

Prevention

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

P272 Contaminated work clothing should not be allowed out of the workplace.

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

P273 Avoid release to the environment.

Response

P302+P352 IF ON SKIN: Wash with plenty of water/...

P333+P317 If skin irritation or rash occurs: Get medical help.

P321 Specific treatment (see ... on this label).

P362+P364 Take off contaminated clothing and wash it before reuse.

P391 Collect spillage.

Storage

none

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:	N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine
Common names and synonyms:	N-(1-ethylpropyl)-2,6-dinitro-3,4-xylidine
CAS number:	40487-42-1
EC number:	254-938-2
Concentration:	100%

SECTION 4: First aid measures

Description of necessary first-aid measures

If inhaled

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

Following skin contact

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

Following eye contact

Rinse with pure water for at least 15 minutes. Consult a doctor.

Following ingestion

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

Most important symptoms/effects, acute and delayed

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: Inhalation of material may be harmful. Contact may cause burns to skin and eyes. Inhalation of Asbestos dust may have a damaging effect on the lungs. Fire may produce irritating, corrosive and/or toxic gases. Some liquids produce vapors that may cause dizziness or suffocation. Runoff from fire control may cause pollution. (ERG, 2016)

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 if necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on the 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. Poisons A and B

SECTION 5: Firefighting measures

Suitable extinguishing media

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: **SMALL FIRE:** Dry chemical, CO₂, water spray or regular foam. **LARGE FIRE:** Water spray, fog or regular foam. Do not scatter spilled material with high-pressure water streams. Move containers from fire area if you can do it without risk. Dike fire-control water for later disposal. **FIRE INVOLVING TANKS:** Cool containers with flooding quantities of water until well after fire is out. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. **ALWAYS** stay away from tanks engulfed in fire. (ERG, 2016)

Specific hazards arising from the chemical

Excerpt from ERG Guide 171 [Substances (Low to Moderate Hazard)]: Some may burn but none ignite readily. Containers may explode when heated. Some may be transported hot. For UN3508, be aware of possible short circuiting as this product is transported in a charged state. (ERG, 2016)

Special protective actions for fire-fighters

Wear self-contained breathing apparatus for firefighting if necessary.

SECTION 6: Accidental release measures

Personal precautions, protective equipment and emergency procedures

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

Environmental precautions

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must

be avoided.

Methods and materials for containment and cleaning up

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.

SECTION 7: Handling and storage

Precautions for safe handling

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

Store above 40 deg F. Extended storage at temperatures less than 40 deg F can result in the formation of crystals on the bottom of the container. If crystallization does occur, store the container on its side at room temperature (70 deg F) and rock occasionally until crystals redissolve. Do not store near food or feed products.

SECTION 8: Exposure controls/personal protection

Control parameters

Occupational Exposure limit values

no data available

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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

Skin protection

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

Thermal hazards

no data available

SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Pendimethalin is an orange-yellow crystals. Non corrosive. Used as an herbicide.
Colour:	Orange-yellow crystal solid
Odour:	Faint, nutty odor
Melting point/freezing point:	56-57°C
Boiling point or initial boiling point and boiling range:	330°C
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	208.4°C
Auto-ignition temperature:	no data available

Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	Soluble in most organic solvents
Partition coefficient n-octanol/water:	log Kow = 5.20
Vapour pressure:	9.4X10-6 mm Hg at 25 deg C
Density and/or relative density:	1.17
Relative vapour density:	no data available
Particle characteristics:	no data available

SECTION 10: Stability and reactivity

Reactivity

no data available

Chemical stability

Very stable in storage. Stable to acids and alkalis. Slowly decomposed by light.

Possibility of hazardous reactions

A dinitroaniline derivative.

Conditions to avoid

no data available

Incompatible materials

no data available

Hazardous decomposition products

When heated to decomposition it emits toxic fumes of nitroxides.

SECTION 11: Toxicological information**Acute toxicity**

Oral: LD50 Rat oral 1050 mg/kg

Inhalation: no data available

Dermal: no data available

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

Cancer Classification: Group C Possible Human Carcinogen

Reproductive toxicity

no data available

STOT-single exposure

no data available

STOT-repeated exposure

no data available

Aspiration hazard

no data available

SECTION 12: Ecological information**Toxicity**

Toxicity to fish: LC50; Species: *Lepomis macrochirus* (Bluegill sunfish); Concentration: 0.199 ppm for 96 hr 93.2% a.i. /Conditions of bioassay not given

Toxicity to daphnia and other aquatic invertebrates: LC50; Species: *Daphnia magna* (water flea); Concentration: 0.28 ppm for 48 hr /Conditions of bioassay not given

Toxicity to algae: no data available

Toxicity to microorganisms: no data available

Persistence and degradability

AEROBIC: Using water from two nursery recycling ponds, pendimethalin exhibited first-order half-lives of 26.9-37.4 days at 10 deg C in non-sterile water and 137.5-183.4 days in sterile water(1); at 22 deg C, the first-order half-lives were 16.4-29.1 days in non-sterile water and 71.4-121.0 days in sterile water(1). A soil degradation study using an agro-soil from Iowa found virtually no pendimethalin biodegradation over a 160-day period(2); it was thought that pendimethalin desorption from the soil was very difficult resulting in no bioavailability(2). The persistence of pendimethalin was studied in non-flooded and flooded nonsterile and sterile sandy loam soil (0.35% organic carbon, pH 8.2%) at 30 deg C over 90 days(3). The degradation was first order with half-lives of 52.2 and 33.4 days in nonsterile nonflooded and flooded soil, respectively, and 66.9 and 44.9 days in sterile nonflooded and flooded soil, respectively(3). Therefore degradation is faster in flooded than in nonflooded soil. While the herbicide was more persistent in nonsterile than sterile soil, only 11-14% of the degradation over 90 days could be attributed to microbial activity. The formation of two major metabolites, N-(1-ethylpropyl)-3,4-dimethyl-2-nitrobenzene-1,6-diamine and 3,4-dimethyl-2,6-dinitroaniline indicate that under aerobic conditions N-dealkylation and reduction of the less hindered nitro groups are primary transformation mechanisms. The same products were formed when pendimethalin was incubated with enriched cultures of soil fungi(4). Under flooded conditions, the sole product was N-(1-ethylpropyl)-5,6-dimethyl-7-nitrobenzimidazole which is formed

through the intermediate, 6-aminopendimethalin in the presence of a source of carbon(3). Presumably, the source of carbon is needed to supply the carbon atom on the benzimidazole ring(SRC). Statements were also made by the investigators without any supporting data that complete degradation of pendimethalin in flooded soil could occur in four and even one day, as a result of which short periods of excessive rainfall could cause unexpectedly rapid dissipation of pendimethalin and the formation of alternate degradation products(3). No discussion of possible mechanisms was presented for the comparable amounts of degradation in sterile soil(SRC).

Bioaccumulative potential

A bioconcentration study using USEPA guideline 165-4 (OPPTS 850.1730), Bluegill fish (*Lepomis macrochirus*) and a 28-day exposure period determined a pendimethalin BCF value of 5,100(1). According to a classification scheme(2), this BCF suggests the potential for bioconcentration in aquatic organisms is very high(SRC). ¹⁴C-Pendimethalin-treated soil (1 and 10 ppm) was added to a model ecosystem containing 16 L of water 400 g of soil, snails, fish, algae, and daphnids and monitoring over 30 days(3); snails reached their peak ¹⁴C level between days 7 and 15; while 50% of the radioactivity was pendimethalin on day-1, <1% was so by day-15; fish reached their peak ¹⁴C level on day-1 and thereafter levels declined paralleling that of ¹⁴C in water; while 76% of the radioactivity was pendimethalin on day-1, this decreased to 22% by day-30; these data suggest that fish preferentially accumulated pendimethalin over more polar metabolites and degraded it more slowly than snails; algae accumulated ¹⁴C slowly over the 30-day experiment and daphnia reached a ¹⁴C plateau between day-7 and day-15, but this depurated within 10 days in fresh water; the maximum ¹⁴C BCF (as pendimethalin) ranged from 190 (algae) to 312 (fish)(3). The BCF of pendimethalin in a sea nettle (*Chrysaora quinquecirrha*) was 0.42 after 16 hrs(4).

Mobility in soil

Batch equilibrium adsorption tests using nine different soils (organic carbon ranging from 0.44% to 2.91%) determined pendimethalin Koc values ranging from 7,011-43,863(1). Koc values in five different soils ranged from 6,500-29,400 with a median/recommended Koc value of 13,400(2). According to a classification scheme(3), these Koc values suggest that pendimethalin is expected to be immobile in soil. A four year field study in a sandy loam soil from 2003-2007 found no pendimethalin detected below a 10 cm soil depth(4). A field study in turfgrass land of loamy sand soil observed a low runoff and leaching of applied pendimethalin(5); runoff was highest following the first rainfall and decreased exponentially thereafter(5). Koc values of 10,200 and 22,000 were observed using two sediments from a nursery recycling pond(6).

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: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

UN Proper Shipping Name

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Transport hazard class(es)

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (For reference only, please check.)

Packing group, if applicable

ADR/RID: Not dangerous goods. (For reference only, please check.)
IMDG: Not dangerous goods. (For reference only, please check.)
IATA: Not dangerous goods. (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

Not Listed.

China Catalog of Hazardous chemicals 2015

Not Listed.

New Zealand Inventory of Chemicals (NZIoC)

Listed.

(PICCS)

Not 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/>

Disclaimer: The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. We as supplier shall not be held liable for any