**LingLan Biopharmaceutical Co.,Ltd**
**ADD: Beijing city,ChaoYang district,JingTai Mansion 2-019**

# Certificate Of Authenticity

**COA Number** : 20170805 **COA Date**: 20170805 **Validity**: 180 days

## Nitroethane Basic information

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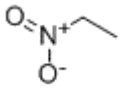
| Product Name: | Nitroethane |
| Synonyms: | 1-Nitroethane;C2H5NO2;Ethane,nitro-;Nitroetan;nitroetan(polish);nitro-ethan;Nitroparaffin;NITROETHANE |
| CAS: | **79-24-3** |
| MF: | C2H5NO2 |
| MW: | 75.07 |
| EINECS: | 201-188-9 |
| Product Categories: | Organics;Solvent |
| Mol File: | 79-24-3.mol |



## Nitroethane Chemical Properties

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| Melting point | -90 °C |
| Boiling point | 114-115 °C(lit.) |
| density | 1.045 g/mL at 25 °C(lit.) |
| vapor density | 2.58 (vs air) |
| vapor pressure | 15.6 mm Hg ( 20 °C) |
| refractive index | *n*20/D 1.391(lit.) |
| Fp | 87 °F |
| storage temp. | Flammables area |
| solubility | acetone: soluble(lit.) |
| pka | 8.5(at 25℃) |
| PH | 6 (1g/l, H2O, 25℃) |
| explosive limit | 3.4%(V) |
| Water Solubility | 4.6 g/100 mL (20 °C) |

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| Merck | 14,6597 |
| BRN | 1209324 |
| Stability: | Stability Contact with a variety of materials may cause fire or explosion, especially if heated. Incompatible with amines, strong acids, strong oxidizing agents, combustible materials, metal oxides, strong bases, alkalies. |
| CAS DataBase Reference | 79-24-3(CAS DataBase Reference) |
| NIST Chemistry Reference | Ethane, nitro-(79-24-3) |

## Safety Information

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| Hazard Codes | T,Xn |
| Risk Statements | 45-10-20/22-68 |
| Safety Statements | 9-23-41-25-45-36/37-53 |
| RIDADR | UN 2842 3/PG 3 |
| WGK Germany | 2 |
| RTECS | KI5600000 |
| TSCA | Yes |
| HazardClass | 3 |
| PackingGroup | III |
| Hazardous Substances Data | 79-24-3(Hazardous Substances Data) |

## Nitroethane Usage And Synthesis

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| Summary | It is colorless oily liquid, with unpleasant odor. The molecular weight is 75.07, the melting point is-50℃. The boiling point is 114 ℃ to 114.8 ℃. The relative density is 1.0528. The refractive index is 1.3917. The flash point is 30 ℃. It can be soluble in methanol, ethanol, ether, chloroform and aqueous alkali miscible, soluble in water. The solubility in water is 4.5mL/100mL(20℃), but the water solubility in this product is 0.9mL/100mL (20 ℃). Steam and air can form explosive mixtures, explosion limit is 3%~5% (in volume). Toxic! Due to chemical properties of nitro ethane is stable, can be used as nitrocellulose and cellulose acetate, vinyl and alkyd resin, wax, grease, fat and dye solvent, is also used as a propellant and fuel additives, pharmaceutical and organic synthesis intermediates. It can be prepared by direct gas phase nitration of ethane or produced by the effect of α-acid chloride and sodium nitrite.<br>The above information is Chemicalbook Hanya edited. |
| Nitromethane | Nitromethane is the simplest organic nitro compounds, is a colorless oily with a faint aromatic smell of transparent liquid at room temperature, with a larger polar, flammable, poisonous, and explosive. It can be used as fuel. It can be miscible with ethanol, acetone and ethyl ether, is a good solvent and extractant. At the same time, because the nitro α-hydrogen has strong activity, nitromethane is the chemical and organic synthesis of common materials for preparation of drugs, pesticides, explosives, dyes and fibers. |

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| | Nitromethane is a synthesis of carbon sub in organic synthesis. By the influence of nitro suction electronic effect, hydrogen of carbon has acidity, and react with alkali to deprotonate. The generation of negative ions of carbon can with aldehydes occurs 1,2 addition generateβ-hydroxy nitro compounds , if loss of water is generated nitro olefin. The reaction is called as Henry reaction. As negative ions of carbon nucleophiles to body, nitromethane can be occurrence conjugate addition with α,β-unsaturated carbonyl compounds under the catalysis of alkali , which is said Michael addition reaction.<br>In Industry, we can take nitric acid gas phase (350-450℃) nitrification propane method for preparation of the nitro methane and other low-level nitro compounds, such as nitroethane, 1-nitropropane and 2-nitropropane and so on. The reaction is exothermic reaction, free radical mechanism, intermediates is alkyl nitrite homolytic production of free radical CH3CH2CH2O type. Most of them were unstable, prone to C-C bond cleavage, so the reaction obtained a nitro compounds and lower mixture of nitro compounds. |
| Nucleophilic addition reaction | Under the cataelysis of alkali, the reaction of nitro alkanes with aldehyde and ketone generated aldehyde condensation to obtain β-nitro alcohols, which was eliminated gradually, and obtained α,β-unsaturated nitro alkanes, which is called Henry.<br>Because nitro has electron withdrawing effect in nitroethane, and nitro adjacent carbon of hydrogen becomes lively, strip of hydrogen is a negative ion of carbon. And aldehyde carbon of benzaldehyde influenced by oxygen, with some positively charged, so it can be attacked, nitroethane and benzaldehyde react to 1-phenyl-2-nitro-1-propanol, the latter soon remove a molecule of water to obtain 1-phenyl-2-Nitro propylene. |
| Preparation of antihypertensive drug methyldopa | The vanillin with dimethyl sulfate methylate to veratraldehyde, then with nitroethane condensation to obtain the 1-(2-nitro-propenyl) 3', 4'-dimethoxy benzene, by reduction with iron powder and hydrolyzed generation to 3 ', 4'-dimethoxy benzene acetone and by cyclization, ring opening, hydrolysis reaction to get methyldopa DL, splitting the levorotatory to obtain an antihypertensive drug methyldopa. |
| Dangerous situation | (1) It is toxic, inhalation and ingestion of this product can cause poisoning; the high fever will be decomposed, decomposition products are highly toxic.<br>(2) flammable, secondary combustion risk, ignition is 415 ℃. Vapor can form explosive mixtures with air, lower limit of explosion limit is 3.4%, high limit is unknown. Rapid heating to a high temperature may cause an explosion; in the solid sealed conditions, the effect of strong explosion also exploded. Air in the allowable concentration of the United States is 100 ppm (310mg/m3). |
| Harmful effects and toxic symptoms | Contacting with the skin can cause contact dermatitis, inhalation of high concentration has effect of anesthesia. |
| first aid | If the chemicals into the eyes, rinse with water immediately; in case of contacting with skin, rapid wash with soap and water; If a large number of inhalation, immediately moved away from the scene to fresh air. When necessary, carry out artificial respiration; If mistakenly swallowed, emetic, gastric lavage, give the medical gaze, symptomatic treatment; severe cases, do not induce vomiting immediately , should be sent to hospital for treatment. |
| Protection measures | Production site should strengthen ventilation, equipment should be sealed. Operation should wear suitable protective clothing, to prevent skin repeatedly or prolonged contact. Also need to wear a mask or respirator isolation to prevent inhalation of smoke and gas. If the skin of workers is wet or contaminated and should be a quick rinse. If work clothes was wet or contaminated, immediately remove, in order to avoid fire hazard. |

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| keep in storage | Using glass bottles or drum costumes to prevent mechanical damage; used in containers shall not again for holding. It is best to use open or attached to build warehouse in outdoor storage, must be placed within the flammable liquids designed library. And other flammable liquid or gas should be isolated. Explosive and dangerous work prohibited in the warehouse district around. With the oxidant separated. |
| chemical property | Colorless transparent oily liquid. Insoluble in water, immiscible with ethanol, ether, chloroform and alkali solution. |
| Uses | 1.Used as industrial solvents and pharmaceutical intermediates, explosives, rocket fuels, etc.<br>2.Used as solvent, pharmaceutical intermediate, explosive, rocket fuel and analytical reagent.<br>3.Used as a solvent, also used in organic synthesis.<br>4.Solvents. Organic synthesis. |
| Production method | In Industry, mainly uses low carbon alkane direct vapor phase nitration method for production. With methane as raw material, only production of nitromethane; ethane as raw material, can prepare nitromethane and nitroethane two products; with propane as raw materials, can prepare the methane, nitroethane and 1-nitropropane, 2-nitropropane four products. In terms of ethane and propane as raw materials, you can through changes condition to change the proportion of products. |
| category | Flammable liquid |
| Toxicity grading | poisoning |
| Chemical Properties | colourless oily liquid with an unpleasant odour |
| acute toxicity | Oral administration of LD50: 1100 mg/kg in rats; oral administration of 860 mg/kg of LD50: in mice |
| Definition | ChEBI: A nitroalkane that is ethane substituted by a nitro group. |
| Explosive hazard characteristics | In case of thermal explosion.<br>Flammable risk characteristics in case of fire, high temperature, oxidation of flammable; heat decomposition of toxic nitrogen oxide gas. |
| Storage and transportation characteristics | warehouse ventilation low temperature drying and oxidation agent, alkali and hydrocarbons separately. |
| Fire extinguishing agent | dry powder, dry sand, carbon dioxide, foam, 1211 fire extinguishing agent. |
| Occupation standard | TWA 310 mg/cubic meter |
| General Description | A colorless oily liquid with a pleasant odor. Flash point of 82°F. Decomposes above 350°F. Density 1.052 g / cm3. Vapors much heavier than air. and insoluble in water. Vapors may irritate skin, eyes and mucous membranes. Produces toxic oxides of nitrogen during combustion. Used as a propellant and as a solvent. |
| Air & Water Reactions | Highly flammable. Water soluble. |
| Reactivity Profile | The nitroparaffins, nitromethane, nitropropane, etc. form salts with inorganic bases such as calcium hydroxide. The dry salts are explosive [Chem. Eng. News 30:2344. 1952]. Nitroethane and other nitro compounds are mild oxidizers and should not be heated with easily oxidizable hydrocarbons under confinem |

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| | ent [Chem. Eng. News 30:2344. 1940]. |
| Health Hazard | Inhalation causes moderate irritation of respiratory tract. Ingestion causes irritation of mouth and stomach. Contact with liquid causes irritation of eyes and mild irritation of skin. |
| Fire Hazard | Special Hazards of Combustion Products: Toxic oxides of nitrogen may form in fire. |

## Nitroethane Preparation Products And Raw materials

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| Raw materials | Nitromethane-->2-Nitropropane-->1-Nitropropane |
| Preparation Products | Nitromethane-->2-(8-BROMO-2,3,6,7-TETRAHYDRO-BENZO[1,2-B:4,5-B']DIFURAN-4-YL)-1-METHYL-ETHYLAMINE-->2-Nitropropane-->Methylthioacetaldoxime-->3,5-DIMETHYLISOXAZOLE-4-CARBONYL CHLORIDE-->S-(-)-Carbidopa-->3,5-DIMETHYLISOXAZOLE-4-CARBOXYLIC ACID-->2-Fluorophenylacetone-->3-Methyl-4-isoxazolecarboxylic acid-->Methyldopa-->1-Nitropropane -->2-Fluoroisonicotinic acid-->ETHYL 3,5-DIMETHYLISOXAZOLE-4-CARBOXYLATE-->2-Methoxyphenylacetone-->2-Fluoropyridine-6-carboxylic acid-->DL-Norephedrine hydrochloride |

## Nitroethane Certificate Of Authenticity

| Items | Limits |
|---|---|
| Appearance | Conform |
| Assay | 99.9% |
| Density | 1.045 |
| Refractive index | 1.391 |
| Boiling point | 114°C |
| Water | 0.036% |
| Total impurities | 0.23% |
| Single impurity | 0.04% |
| Conclusion | Conform |
| Appearance | The results conforms with enterprise standard. |

*Issued :*
*Date:*

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