ANGUS® CHEMICAL COMPANY

Key Performance Advantages

- Excellent intermediate and specialty solvent
- Efficient chemical intermediate for organic synthesis

NITROETHANE [NE™]

$CH_3CH_2NO_2$
CAS Reg. No. 79-24-3
EINECS No. 2011889

Nitroparaffins possess a combination of physical and chemical properties which make them essential for many diversified applications. Nitroethane (NE™) has found its greatest use as a synthetic intermediate and specialty solvent.

Typical Properties

The following are typical properties of nitroethane. They are not to be considered product specifications.

Nitroethane content % by wt*	>98.0
Total nitroparaffins, % by wt*	>99.0
Water, % by wt	<0.2
Color, APHA	<20
Distillation range @ 1 atm (90% min)	112-116˚C/223-240˚F
Vapor density (air = 1)	2.58
Specific gravity @ 25/25˚C	1.045
Change of density with temperature, 0-50˚C, g/(mL ˚C)	0.0012
Weight per US gallon @ 20˚C/68˚F, lb	8.75
Flash point, Tag open cup	41˚C/106˚F
Flash point, Tag closed cup	30˚C/87˚F
Lower limit of flammability, % by vol (@ 30˚C)	3.4
Upper limit of flammability (177˚C)	40
Ignition temperature	414˚C/777˚F
Evaporation rate (n-butyl acetate = 100)	121
Evaporation number (diethyl ether = 1)	11

*Determined by gas chromatograph

Physical Properties of Nitroethane

Molecular weight (calculated)	75.07
Boiling point @ 760 mm Hg, ˚C	114.07
Vapor pressure @ 25˚C, mm Hg	20.93
Freezing point, ˚C	- 89.52
Density @ 20˚C, g/mL **@ 30˚C, g/mL**	1.051 1.039
Coefficient of expansion per ˚C **Per ˚F**	0.00112 0.00062
Refractive index, nD @ 20˚C **@ 30˚C**	1.39193 1.38754
Surface tension @ 20˚C, dynes/cm	32.66
Viscosity @ 20˚C, cp **@ 30˚C, cp**	0.677 0.602
Heat of combustion (liq.) @ 25˚C, kcal/mole	- 325.6
Heat of vaporization (liq.) @ 25˚C, kcal/mole **@ bp, kcal/mole**	9.94 9.08
Heat of formation (liq.) @ 25˚C, kcal/mole	- 33.9
Specific heath @ 25˚C, cal/(mole ˚C) **@ 25˚C, cal/(g ˚C)**	33.1 0.441
Dielectric constant @ 30˚C	28.06
Dipole moment, μ, **Gas, Debye units** **Liquid, Debye units**	 3.58 3.19
pH of 0.01 M aqueous solution	6.0
Solubility in water @ 20˚C, % by wt **@ 25˚C, % by wt** **@ 70˚C, % by wt**	4.6 4.7 6.6
Solubility of water in NE **@ 20˚C, % by wt** **@ 25˚C, % by wt** **@ 70˚C, % by wt**	 0.9 1.1 3.0
Hydrogen bonding parameter	2.5
Solubility parameter	11.1

Azeotropes with Nitroethane

		Azeotrope	
Compound	**b.p., ˚C**	**Wt % of Compound**	**b.p., ˚C**
Propyl nitrate	110.5	<79	<109.6
Propyl alcohol	97.2	68.2	94.5
Isopropyl alcohol	82.4	89.4	81.8
1-Bromobutane	101.5	75	96.0
1-Bromo-2-methylpropane	91.4	90	89.5
Butyl alcohol	117.8	45	107.7
Sec-butyl alcohol	99.5	72.4	97.2
t-butyl alcohol	82.4	95.5	82.2
Isobutyl alcohol	108.0	<60	<102.5
1-Bromo-3-methylbutane	120.6	<45	<108.5
Amyl alcohol	138.2	<17	<137.8
t-amyl alcohol	102.4	<70	<98.6
Isoamyl alcohol	131.9	22	112
Methylcyclopentane	72	<96	<71.2
4-Methyl-2-pentanone	116	-	<113
Ethyl butyrate	121.5	<27	<113.7
Ethyl isobutyrate	110.1	73	108.5
Isobutyl acetate	117.4	40	112.5
Isopropyl sulfide	120.5	<40	<110.9
Toluene	110.8	75	106.2
Methylcyclohexane	101.2	70	90.8
n-Heptane	98.4	72	89.2
2,5-Dimethylhexane	109.4	<38	<96.9
Acetic acid	114.2	30	112.4
Water	100	28.5	87.2
Ethyl alcohol	78.3	87.4	78

Nitroethane is reported not to form azeotropes with benzene or methanol.

Uses as a Solvent

Nitroethane has solvency properties of particular interest for specialty applications.

It is an excellent solvent for a wide variety of organic compounds and for resins, such as acrylic and vinyl resins, used in coatings and inks. It can be used as a solvent for the extraction of rosin from wood, for example.

Separation systems based on nitroethane have been devised and studied extensively for fractionating petroleum distillate oils and for the dewaxing of diesel fuels.

Nitroethane is useful in inhibiting the decomposition of halogenated hydrocarbon solvents, thus preventing their release of acids. The addition of a small amount of nitroethane to these useful degreasing solvents and refrigerants eliminates their corrosive attack on metals.

Some inorganic materials are also soluble in nitroethane. For instance, nitric acid and uranyl ions will dissolve in nitroethane and with it can be extracted from aqueous media and purified. Nitroethane is a solvent for anhydrous aluminium chloride, which forms a 1:1 complex with nitroethane. This complex is active as a Friedel-Crafts catalyst.

Use in Synthesis

Nitroethane is most useful as a chemical intermediate for organic synthesis.

Because of the acidity of its α-hydrogen atoms, nitroethane undergoes many base-catalyzed addition and condensation reactions. Such reactions are convenient for the introduction of nitro groups into molecules. The first step in the synthesis of the insecticide Prolan, for instance, is the condensation of nitroethane with chlorobenzaldehyde.

Nitro compounds are readily reduced to the corresponding amino compounds. 2-nitro-2-methyl-1, 3-propanediol (NMPD), formed by the reaction of two moles of formaldehyde with nitroethane, can be reduced to 2-amino-2-methyl-1,3-propanediol (AMPD). Detailed discussions of the chemistry of these two classes of derivatives—the nitrohydroxy compounds and the aminohydroxy compounds—are in ANGUS Nitro Alcohols and ANGUS Primary Amino Alcohols Technical Data Sheets, respectively.

Dimethoxyphenylacetone, a raw material for the manufacture of α-methyldopa, is readily synthesized by reaction of 3,4-dimethoxybenzaldehyde with nitroethane, followed by catalytic hydrogenation and hydrolysis.

The insecticide methomyl is conveniently prepared by the treatment of the potassium salt of nitroethane with methyl mercaptan and methanol.

For further, more detailed information on the uses of nitroethane in synthesis, please contact ANGUS.

Chemical Reactions

Chemical reactions can be found in ANGUS' Nitroparaffin Chemistry Guide. A number of review articles which provide additional detailed information on nitroparaffin chemistry are available by request.

Toxicity

Oral

The acute oral LD50 for nitroethane in the Sprague-Dawley strain of rat is estimated to be 1625 ± 193 mg/kg of body weight. Thus, nitroethane is classified by toxicologists as slightly toxic following oral administration, since it is within the toxic range of 500 to 5000 mg/kg. Should accidental ingestion occur, promptly induce vomiting.

Dermal Absorption

In a dermal application to rabbits, a nitroethane dose of 2000 mg/kg of body weight was not absorbed in lethal amounts. There were no deaths nor any signs of significant gross toxicity.

Eye and Skin Irritation

A dose of 0.1 mL of undiluted nitroethane instilled into the eyes of rabbits produced no significant degree of toxicity or irritation. Likewise, the product was nonirritating to the abraded and unabraded skin of rabbits. Prolonged or frequently repeated exposure may cause defatting and drying of the skin in a manner similar to that experienced with most other organic solvents.

If nitroethane is splashed in the eyes, flush eyes well with water. In case of accidental spillage on skin and clothing, wash well with soap and water and change to clean clothing.

Vapor Inhalation

The American Conference of Governmental Industrial Hygienists has established a threshold limit value for nitroethane of 100 ppm (310 mg/m3) as a time-weighted average concentration for an 8-hour workday and a 40-hour workweek. This value has been adopted as a permissible limit by the Occupational Safety and Health Administration, US Department of Labor (cf.29 CF R 1910.1000). If exposure limit is anticipated, a self-contained breathing apparatus should be used. Remove an exposed individual to fresh air at once; get medical attention.

Vapor-inhalation studies employing 6-hour daily exposure periods show that a concentration of nitroethane of 550 ppm (1552 mg/m^3) is nonlethal to rats following 12 repeated exposures during a 21-day period.

Rats survived five 6-hour inhalation sessions at a vapor concentration of 2200 ppm (6.8g/m^3) with no noticeable difficulty.

Nitroethane is fatal to rats in 6-7 hours during the course of exposure to an atmosphere containing 13,000 ppm.

Coulston et al. exposed male and female Long Evans rats to vapors of nitroethane at 0, 100, or 200 ppm in air, 7 hours per day, 5 days per week for 2 years. Rats found dead or sacrificed moribund were thoroughly examined for gross abnormalities and tissues retained for microscopic evaluation. After 2 years, all surviving rats were sacrificed. Blood samples were obtained for hematology and serum chemistry studies. All rats were examined histopathologically.

Exposure to nitroethane had no pharmacologic effects, nor was there any effect on mortality of rats of either sex. There were no significant effects of exposure on hematology, clinical chemistry or organ weights. In comparison to the control, no significant difference was observed in the non-neoplastic or neoplastic pathology related to exposure to nitroethane.

Metabolic Studies
Nitroethane, when administered orally or intravenously to rabbits, is partially excreted unchanged by the lungs. The amount of nitroethane found in tissues decreases at a fairly rapid rate. Metabolic products of nitroethane appear to include acetaldehyde and nitrite.

Intraperitoneal injection of nitroethane at a dose of 1.1g/kg in rats was not fatal, whereas 1.6 g/kg caused death in 10-15 hours. Nitroethane was recovered from the liver and exhaled air; nitrites were found in the heart, lung, kidney, and spleen tissues and in urine. Methemoglobinemia may be a consequence associated with these nitrites.

Precautionary Labeling

Labels for **NE** bear these caution statements:

WARNING! FLAMMABLE.

Keep away from heat, sparks, and flame.
Use only with adequate ventilation.
Avoid prolonged breathing of vapor.
Keep container closed.

Dry salts formed with strong alkalis may be ignitable; keep them away from heat, sparks, and flame.

After this container has been emptied, it may contain explosive vapors; observe all warnings and precautions listed for this product. Do not cut, puncture, or weld on or near this container.

In case of:

FIRE - use water spray, foam, or CO_2; use only dry chemical, tri-class extinguishers approved for Class ABC fires.

SPILL - flush spill area with water spray.

FOR INDUSTRY USE ONLY

Storage and Handling

Nitroethane should be handled in a manner similar to that of any volatile organic solvent. Avoid prolonged breathing of nitroethane vapors, and use only with adequate ventilation. Keep containers closed. In case of spills, flush spill area with water spray but not into sewers where vapors may be ignited.

Because it has a flash point of 30˚C/87˚F by Tag closed cup, nitroethane is considered flammable under the definitions of the US Department of Transportation. Keep it away from heat, sparks and flame. Use nonsparking tools when opening containers.

Water spray, foam or CO_2 can be used to control and extinguish burning nitroethane. Use dry chemical triclass extinguishers (those containing only ammonium phosphate and rated for ABC fires) on small nitroethane fires. Dry chemical extinguishers which contain sodium or potassium bicarbonate are not rated for use with class A fires. Such extinguishers only appear to put out nitroethane fires when first applied, but later contribute to reignition. With all chemical fires, self-contained breathing apparatus should be worn when fighting large fires.

For detailed information on materials of construction, storage tanks, pumps, piping, valves, hoses, and polymers, consult one of the ANGUS Technical Data Sheets on the nitropropane solvents (Nipar S-10 or Nipar S-20 Nitropropane Solvent)

Between 80-90˚C/176-194˚F, nitroethane becomes capable of sustaining a high-order detonation. Initiation of such a detonation is difficult and requires an extreme shock, such as that provided by a high explosive booster. Intense heating under heavy confinement can also initiate detonation. For these reasons, operations in which undiluted nitroethane is heated to temperatures exceeding 80˚C/176˚F should be avoided if possible. If processes involving high temperatures are unavoidable, the precautions developed for handling nitromethane can be used to reduce risk (see ANGUS Nitromethane Technical Data Sheet). When allowed to react with alkalis, such as sodium hydroxide, nitroethane forms nitronate salts. When dry, such salts may be ignitable from static electricity or other spark sources. The dry salts also can decompose violently if confined and subjected to elevated temperatures (e.g., 180˚C/356˚F for the sodium salt). Thorough testing should be carried out on the specific product before any attempt is made to produce, use, or ship the dry salts on a large scale. Do not use caustic soda or lye to clean equipment containing nitroethane unless it is thoroughly flushed with water as a final step in the cleaning.

When emptied, drums which contained nitroethane should be cleaned for reuse by filling to overflowing with water followed by thoroughly rinsing several times with water. Do not cut, puncture or weld any drum unless it has been cleaned.

Shipping and Packing

Nitroethane is classified as a Class 3 (Flammable liquid) in the transport regulations issued by the US Department of Transportation (49 CFR) and the International Air Transport Association (IATA). It is a Class 3.3 in the International Maritime Dangerous Goods (IMDG) Code.

The bill of lading description by ANGUS is:

NITROETHANE,3,UN2842,III. IN CASE OF EMERGENCY USE ANGUS GUIDE 8 ATTACHED LACQUER SOLVENT, NOU. NMFC ITEM 149980 SUB 2 CLASS 55. TRADE NAME = NE

Shipping containers	Net Wt.	Gross Wt.
5-gallon steel drum	43 lb	48 lb
55-gallon steel drum	475 lb	513 lb

Product Stewardship

ANGUS encourages its customers to review their applications of ANGUS products from the standpoint of human health and environmental quality. To help ensure that ANGUS products are not used in ways for which they are not intended, ANGUS personnel will assist customers in dealing with environmental and product safety considerations. For assistance, product Safety Data Sheets, or other information, please contact your ANGUS representative at the numbers provided in this document. When considering the use of any ANGUS product in a particular application, review the latest Safety Data Sheet to ensure that the intended use is within the scope of approved uses and can be accomplished safely. Before handling any of the products, obtain available product safety information including the Safety Data Sheet(s) and take the necessary steps to ensure safety of use.

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