n-PROPYL ACETATE

PRODUCT IDENTIFICATION

CAS NO. 109-60-4 EINECS NO. 203-686-1

FORMULA CH3COOCH2CH2CH3

MOL WT. 102.13 H.S. CODE 2915.39

TOXICITY

SYNONYMS 1-Propyl Acetate; Acetic acid, propyl ester;

1-Acetoxypropane; propyl acetate; n-Propyl ethanoate; Acetate de propyle normal; Octan propylu; Propyl ethanoate; Propylester kyseliny octove; Propylacetat; Acetato de propilo; Acétate de propyle;

DERIVATION CLASSIFICATION

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE clear liquid

MELTING POINT -96 C
BOILING POINT 101 - 102 C
SPECIFIC GRAVITY 0.88 - 0.89

SOLUBILITY IN WATER Slightly soluble (Soluble in most organic solvents)

Hq

VAPOR DENSITY

AUTOIGNITION 450 C

NFPA RATINGS Health: 1; Flammability: 3; Reactivity: 0

REFRACTIVE INDEX 1.384 FLASH POINT 10 C

STABILITY Stable under ordinary conditions

GENERAL DESCRIPTION OF SOLVENT

Acetate is the ester that an organic group replaces a hydrogen atom in -OH group of acetic acid through reaction (typically condensation) with alcohols. Condensation is the reaction in which two molecules having -OH groups are joined with eliminating a water molecule from their -OH groups.They are produced by esterification reaction from acetic acid and the corresponding alcohol in the presence of strong acids like sulfuric acid. This reaction is reversible and acetate can be hydrolyzed back into alcohol and acetic acid in the presence of strong bases or strong acid, especially at elevated temperature. The term acetate is also for the salt that one or more of the hydrogen atoms of acetic acid are replaced by one or more cations of the base, resulting in a compound containing the negative organic ion of CH3COO-. Lower acetate is a non-polar to weak polar aprotic solvent which have some solubility portion in water. Its miscibility with water gets higher at elevated temperature. Higher acetates have a low solubility in water and used as extraction solvents for fine chemicals particularly for certain antibiotics. Organic acetates are good solvents for a broad range of resins as they are miscible with almost all common organic liquids. Due to their powerful solvency, high volatility and mild odor, acetates are widely used as solvents for paints, coatings, adhesives, cellulose, plastics, fats, wood stains. Additionally ether acetates series are also widely used as solvents. This surfactant-like structure provides the compatibility between water and a number of organic solvents, and the ability to couple unlike phases. The main products include ethyleneglycol monoethyl ether acetate, ethyleneglycol monobutyl ether acetate, and propyleneglycol monomethyl ether acetate. Aromatic acetates such as benzyl

acetate are also useful solvent. Benzyl acetate has jasmine like odor. Isoamyl acetate has a similar smell to both banana and pear. Acetates have characteristic fruity odor. They are used as component of perfumes and flavorings. They are used as chemical intermediate to manufacture pharmaceuticals, synthetic flavorings, cleaners, and other organic compounds.

Acetate	FORMULA	CAS RN	B.P C
Methyl acetate	CH ₃ COOCH ₃	79-20-9	57 - 58
Ethyl acetate	CH ₃ COOC ₂ H ₅	141-78-6	76.5 - 77.5
Propyl acetate	CH ₃ COOCH ₂ CH ₂ CH ₃	109-60-4	101 - 102
Isopropyl acetate	CH ₃ COOCH(CH ₃) ₂	108-21-4	89
Butyl acetate	CH ₃ COO(CH ₂) ₃ CH ₃	123-86-4	124 - 126
isobutyl acetate	CH ₃ COOCH ₂ CH(CH ₃) ₂	110-19-0	115 - 117
Amyl acetate	CH ₃ COO(CH ₂) ₄ CH ₃	628-63-7	149
Isoamyl acetate	CH ₃ COOCH ₂ CH ₂ CH(CH ₃) ₂	123-92-2	142
Hexyl acetate	CH ₃ COO(CH ₂) ₅ CH ₃	142-92-7	170 - 172
Heptyl acetate	CH ₃ COO(CH ₂) ₆ CH ₃	112-06-1	192 - 193
Octyl acetate	CH ₃ COO(CH ₂) ₇ CH ₃	112-14-1	205 - 211
Nonanyl acetate	CH ₃ COO(CH ₂) ₈ CH ₃	143-13-5	212
Decyl acetate	CH ₃ COO(CH ₂) ₉ CH ₃	112-17-4	272
Undecyl acetate	CH ₃ COO(CH ₂) ₁₀ CH ₃	112-19-6	269 - 271
Lauryl acetate	CH ₃ COO(CH ₂) ₁₁ CH ₃	112-66-3	265
Tridecyl acetate	CH ₃ COO(CH ₂) ₁₂ CH ₃	1072-33-9	
Myristyl acetate	CH ₃ COO(CH ₂) ₁₃ CH ₃	638-59-5	
Pentadecyl acetate	CH ₃ COO(CH ₂) ₁₄ CH ₃	629-58-3	
Cetyl acetate	CH ₃ COO(CH ₂) ₁₅ CH ₃	629-70-9	
Heptadecyl acetate	CH ₃ COO(CH ₂) ₁₆ CH ₃	822-20-8	
Stearyl acetate	CH ₃ COO(CH ₂) ₁₇ CH ₃	822-23-1	
Behenyl acetate	CH ₃ COO(CH ₂) ₂₁ CH ₃	822-26-4	
Hexacosyl acetate	C ₂₈ H ₅₆ O ₂	822-32-2	
Triacontyl acetate	C ₃₂ H ₆₄ O ₂	41755-58-2	
Benzyl acetate	CH ₃ COOCH ₂ C ₆ H ₅	140-11-4	213 - 214
Bornyl acetate	C ₁₂ H ₂₀ O ₂	76-49-3	228 - 231
Isobornyl acetate	C ₁₂ H ₂₀ O ₂	125-12-2	229 - 233
Cyclohexyl acetate	CH3COOC6H11	622-45-7	172 - 173

C V I E C	CDEC		MOITA
$A \cap C \cap$, 3 F F(.IFIL . <i>F</i>	עוכאווי

APPEARANCE	clear liquid
PURITY	99.0% max
ACIDITY	0.01% max
BOILING POINT	98.5 - 102 C
COLOR, APHA	15 max
WATER	0.05% max

TRANSPORTATION

PACKING 170kgs in drum
HAZARD CLASS 3 (Packing Group: II)
UN NO. 1276

OTHER INFORMATION

European Hazard Symbols: F, Risk Phrases: 11, Safety Phrases: 9-16-23-29-33

GENERAL DESCRIPTION OF ACETIC ACID

Acetic acid is the simplest carboxylic acid next to formic acid in which a single hydrogen atom is

attached to the carboxyl group. If a methyl group is attached to the carboxyl group, the compound is acetic acid. Acetic acid is a clear, corrosive, flammable liquid; melting point 16.6 C, boiling point 118 C. Pure acetic acid freezes in ice-like crystal form. So pure acetic acid is called glacial acetic acid, which contains 99.5 - 100.5 % w/w. It is the two-carbon carboxylic acid, and a systematic name is ethanoic acid. It is completely miscible with water, ethyl alcohol and ether, but is insoluble in carbon disulfide. It is a characteristic component of vinegar and an important biochemical intermediate in the form of acetylcoenzyme A, mostly. Most commercial production of virgin synthetic acetic acid is based on methanol carbonylation. Significant volumes of acetic acid are recovered in cellulose acetate operations and lesser quantities during production of polyvinyl alcohol and butyral, peracetic acid, ethylene-vinyl alcohol and acetaminophen and aspirin. Capacity utilization is likely to remain high for the next few years because of good demand for purified terephthalic acid and vinyl acetate monomer.

Vinyl acetate monomer

The largest consumption of acetic acid is as a raw material to produce vinyl acetate by reaction with ethylene and oxygen or with acetylene in the presence of palladium catalyst. Vinyl acetate is polymerized to polyvinyl acetate by itself and to other copolymers with other monomers. Acetate polymers are important resins used in paints, adhesives, plastics and textile finishes.

Acetic anhydride

The next largest consumption of acetic acid is to produce acetic anhydride by condensation reaction of two acetic acid molecules. This chemical is principally used in the manufacture of cellulose acetate having the application as a base for magnetic tape and in the manufacture of textile fibres. Also, it is heated with salicylic acid to produce acetylsalicylic acid (aspirin). It is also used in the manufacture of pigments, dyes, cellulose and pesticides etc.

Solvent

Acetic acid is used as a solvent in the production of terephthalic acid from p-xylene. Terephthalic acid is the raw material for polyester fiber. Terephthalic acid has become a more important raw material for non-fiber field, PET-bottle, PET-film and engineering plastics and as poultry feed additives.

Esters

Considerable quantities of acetic acid are used to manufacture esters such as ethyl and butyl acetate. Acetate esters demonstrate good solvency for many natural and synthetic resins. They are general purpose solvents which are applied commonly in lacquer thinners, wood lacquers and a wide variety of coatings, plasticizer and pharmaceutical fields.

Chloroacetic acid

The stronger acid (chloroacetic acid) is manufactured from acetic acid by reaction with chlorine. Chloroacetic acid reacts with alkali cellulose to produce carboxymethylcellulose (CMC). Chloroacetic acid is the parent material for the production of a series of phenoxy herbicides such as 2,4-dichlorophenoxyacetic acid and 2,4,5-trichlorophenoxyacetic acid.

Acetic acid is used as an acidulant in a wide range of applications from eletroplating to textiles

finishing operation. It is used in the manufacture of materials used in the pharmaceuticals, foods, cosmetics and colorant chemical fields including sorbic acid, dyestuffs and pigments, vitamins, antibiotics, rubber chemicals and flavor & fragrance.