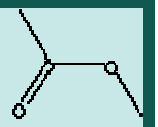
METHYL ACETATE



PRODUCT IDENTIFICATION	
CAS NO.	79-20-9
EINECS NO.	201-185-2
FORMULA	CH_3COOCH_3
MOL WT.	74.08
H.S. CODE	2915.39
TOXICITY	Oral rat LD50: 5000 mg/kg
SYNONYMS	Acetic acid, methyl ester; Methyl acetic ester; Acetate de Methyle (French); Methyl Ester of Monoacetic Acid; Methyl Ethanoate; Methylacetaat (Dutch); Methylacetat (German); Methylester Kiseliny Octove (Czech); Metile (Acetato Di) (Italian); Octan Metylu (Polish);
RAW MATERIALS	
CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	clear liquid
MELTING POINT	-75 C
BOILING POINT	57 - 58 C
SPECIFIC GRAVITY	0.93
SOLUBILITY IN WATER	250 g/l
pH	
VAPOR DENSITY	2.55
AUTOIGNITION	454 C
NFPA RATINGS	Health: 1; Flammability: 3; Reactivity: 0
REFRACTIVE INDEX	
FLASH POINT	< 55 C
STABILITY	Stable under normal conditions

APPLICATIONS

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 CH_3COO^-. 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_3COOCH_3	79-20-9	57 - 58
Ethyl acetate	$CH_3COOC_2H_5$	141-78-6	76.5 - 77.5
Propyl acetate	$CH_3COOCH_2CH_2CH_3$	109-60-4	101 - 102
Isopropyl acetate	$CH_3COOCH(CH_3)_2$	108-21-4	89
Butyl acetate	$CH_3COO(CH_2)_3CH_3$	123-86-4	124 - 126
isobutyl acetate	$CH_3COOCH_2CH(CH_3)_2$	110-19-0	115 - 117
Amyl acetate	$CH_3COO(CH_2)_4CH_3$	628-63-7	149
Isoamyl acetate	$CH_3COOCH_2CH_2CH(CH_3)_2$	123-92-2	142
Hexyl acetate	$CH_3COO(CH_2)_5CH_3$	142-92-7	170 - 172
Heptyl acetate	$CH_3COO(CH_2)_6CH_3$	112-06-1	192 - 193
Octyl acetate	$CH_3COO(CH_2)_7CH_3$	112-14-1	205 - 211
Nonanyl acetate	$CH_3COO(CH_2)_8CH_3$	143-13-5	212
Decyl acetate	$CH_3COO(CH_2)_9CH_3$	112-17-4	272
Undecyl acetate	$CH_3COO(CH_2)_{10}CH_3$	112-19-6	269 - 271
Lauryl acetate	$CH_3COO(CH_2)_{11}CH_3$	112-66-3	265
Tridecyl acetate	$CH_3COO(CH_2)_{12}CH_3$	1072-33-9	
Myristyl acetate	$CH_3COO(CH_2)_{13}CH_3$	638-59-5	
Pentadecyl acetate	$CH_3COO(CH_2)_{14}CH_3$	629-58-3	
Cetyl acetate	$CH_3COO(CH_2)_{15}CH_3$	629-70-9	
Heptadecyl acetate	$CH_3COO(CH_2)_{16}CH_3$	822-20-8	
Stearyl acetate	$CH_3COO(CH_2)_{17}CH_3$	822-23-1	
Behenyl acetate	$CH_3COO(CH_2)_{21}CH_3$	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	$CH_3COOCH_2C_6H_5$	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	$CH_3COOC_6H_{11}$	622-45-7	172 - 173

SALES SPECIFICATION

APPEARANCE	Clear liquid
PURITY (GC)	97.0% , 80.0%
WATER	0.1% max
COLOR (Pt-Co)	10 max

TRANSPORTATION

PACKING	
HAZARD CLASS	3 (Packing Group: II)
UN NO.	1231

OTHER INFORMATION

European Hazard Symbols: F, Risk Phrases: R 11-36-66-67, Safety Phrases: 16-23-29-33
FEMA No: 2676

GENERAL DESCRIPTION OF SOLVENT

Solvent is a substance, usually a liquid, that acts as a dissolving agent or that is capable of dissolving another substance. In solutions of solids or gases in a liquid, the liquid is the solvent. In all other homogeneous mixtures (i.e., liquids, solids, or gases dissolved in liquids; solids in solids; and

gases in gases), solvent is the component of the greatest amount. The minor proportion substances are called solutes. The solvent offers several functions during a chemical reaction. It solves not only the substance that reacts with another one to produce a new set of substances (reactant) but also the compound that supplies the molecule, ion, or free radical, which is considered as the attacking species in a chemical reaction (reagent). The solvent is conductive to collisions between the reactants and reagents to transform the reactants to new products. The solvent also takes roll of temperature control, either to provide the energy of the colliding particles for speedy reaction and to absorb heat in exothermic reaction. The appropriate solvent should be selected based on the inactivity in the reaction conditions, dissolving the reagents as well as reactants, appropriate boiling point and easy removal at the end of the reaction.

Polarity

The most common solvent is water. Other common solvents which dissolve substances that are insoluble (or nearly insoluble) in water are acetone, alcohol, formic acid, acetic acid, formamide. BTX, carbon disulfide, diemthyl sulfoxide, carbon tetrachloride, chloroform, ether, tetrahydrofuran, furfural, hexane and turpentine. They may be classified as polar and non-polar. Polar solvents, like water, have molecules whose electric charges are unequally distributed, leaving one end of each molecule more positive than the other. Usually polar solvent has O-H bond of which water (HOH), (CH_3OH) and acetic acid (CH_3COOH) are examples. Propanol, butanol, formic acid, formamide are polar solvents. Dipolar solvents which contain a C-O solid bond without O-H bond are acetone [$(CH_3)_2C=O$], ethyl acetate ($CH_3COOCH_2CH_3$), methyl ethyl ketone, acetonitrile, N,N-dimethylformamide and diemthyl sulfoxide. Nonpolar solvents, like carbon tetrachloride (CCl_4), benzene (C_6H_6), and diethyl ether ($CH_3CH_2OCH_2CH_3$), have molecules whose electric charges are equally distributed and are not miscible with water. Hexane, tetrahydrofuran and methylene chloride are non-polar solvents. Polar solvents are hydrophilic but non-polar solvents are lipophilic. Polar reactants will dissolve in polar solvents. Non-polar solvents dissolve non-polar compounds best. Oil and water don't mix but separate into two layers. There are three measures of the polarity as "dipole moment", "dielectric constant" and "miscibility with water". Though low dipole moments and small dielectric constants indicates non-polar solvents, sharp boundaries between polar and non-polar solvents are not available. The polarity reflects the balance between a polar component (OH) and a non-polar hydrocarbon component, existing in the same molecule. If hydrocarbon character increases relatively, the polarity decreases. On an operational basis, solvents that are miscible with water are polar.

Polar Protic and Dipolar Aprotic

Protic refers to a hydrogen atom attached to an electronegative atom. Protic solvents can donate an H+ (proton) since they contain dissociable H+, such as hydrogen attached to oxygen as in a hydroxyl group, nitrogen as in a amine group. Examples are water, methanol, ethanol, formic acid, hydrogen fluoride and ammonia. Aprotic solvents don't has O-H bond but a C=O bond typically. Examples are acetone [$(CH_3)_2C=O$] and ethyl acetate ($CH_3COOCH_2CH_3$). Polar protic solvents are useful in S_N1 reaction, while polar aprotic solvents are S_N2 reaction.

Solvents	Boiling point C	Dipole Moment	Dielectric Constant	Density (g/ml)
Polar Protic				
Water	100	1.85	80	0.998
Methanol	68	1.70	33	0.791
Ethanol	78	1.69	24.3	0.789

n-Propanol	97	1.68	20.1	0.803
n-Butanol	118	1.66	17.8	0.810
Formic acid	100	1.41	58	1.21
Acetic acid	118	1.74	6.15	1.049
Formamide	210	3.73	109	1.134
Polar Aprotic				
Acetone	56	2.88	20.7	0.786
Tetrahydrofuran	66	1.63	7.52	0.886
Methyl ethyl ketone	80	2.78	18.5	0.805
Ethyl acetate	78	1.78	6.02	0.894
Acetonitrile	81	3.92	36.6	0.786
N,N-Dimethylformamide	153	3.82	38.3	0.944
Diemthyl sulfoxide	189	3.96	47.2	1.092
Non-Polar				
Hexane	69	-	2.02	0.655
Benzene	80	0	2.28	0.879
Diethyl ether	35	1.15	4.34	0.713
Methylene chloride	40	1.60	9.08	1.326
Carbon tetrachloride	76	0	2.24	1.594