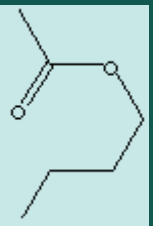
n-BUTYL ACETATE



PRODUCT IDENTIFICATION	
CAS NO.	123-86-4
EINECS NO.	204-658-1
FORMULA	$CH_3COOC_4H_9$
MOL WT.	116.16
H.S. CODE	2915.39
TOXICITY	Oral rat LD50: > 10000 mg/kg
SYNONYMS	Butyl acetate; 1-Acetoxybutane; 1-Butyl acetate; Acetate de butyle (French); Acetic Acid Butyl Ester; Butile (Acetati Di) (Italian); Butyl Ethanoate; Butylacetat (German); Butylacetate; Butylacetaten (Dutch); Butyle (Acetate De) (French); Butylester Kyseliny Octove (Czech); Octan n-Butylu (Polish); Butyl Ethanoate;
DERIVATION	
CLASSIFICATION	

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	clear liquid
MELTING POINT	-106 C
BOILING POINT	126 C
SPECIFIC GRAVITY	0.882
SOLUBILITY IN WATER	Slightly soluble
pH	
VAPOR DENSITY	4
AUTOIGNITION	
NFPA RATINGS	Health: 1; Flammability: 3; Reactivity: 0
REFRACTIVE INDEX	1.394
FLASH POINT	
STABILITY	Stable under normal conditions.

GENERAL DESCRIPTION & 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. 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^-. 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 in the manufacture and in the processing of paints, coatings, adhesives, and printing industry. They have a very low solubility in water and used as extraction solvents for fine chemicals particularly for certain antibiotics. They are also used as components of aroma. They are used as chemical intermediate to manufacture pharmaceuticals, synthetic flavorings, cleaners, and other organic compounds.

SALES SPECIFICATION	
APPEARANCE	Clear liquid
PURITY (GC)	99.0% min
WATER	0.2% max
COLOR (Pt-Co)	15 max

TRANSPORTATION	
PACKING	170kgs in drum
HAZARD CLASS	3 (Packing Group: II)

UN NO.	1123

OTHER INFORMATION

Hazard Symbols: F, Risk Phrases: 10, Safety Phrases: 9-16-33
FEMA No: 2174

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 double 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