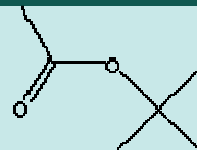


tert-BUTYL ACETATE

PRODUCT IDENTIFICATION

| | |
|------------|--|
| CAS NO. | 540-88-5 |
| EINECS NO. | 208-760-7 |
| FORMULA | CH ₃ COOC ₄ H ₉ |
| MOL WT. | 116.16 |
| H.S. CODE | 2915.39 |
| TOXICITY | Oral rat LD50: > 10000 mg/kg |
| SYNONYMS | Acetic acid, tert-butyl ester; 1,1-Dimethyl ethyl acetate; acetic acid, 1,1-dimethylethyl ester; t-Butyl acetate; |



DERIVATION

CLASSIFICATION

PHYSICAL AND CHEMICAL PROPERTIES

| | |
|---------------------|---|
| PHYSICAL STATE | clear liquid |
| MELTING POINT | |
| BOILING POINT | 97 - 98 C |
| SPECIFIC GRAVITY | 0.9 |
| SOLUBILITY IN WATER | Insoluble (soluble in ethanol, ether) |
| pH | |
| VAPOR DENSITY | 4 |
| AUTOIGNITION | |
| NFPA RATINGS | Health: 1; Flammability: 3; Reactivity: 0 |
| REFRACTIVE INDEX | 1.3853 |
| FLASH POINT | 17 C |
| STABILITY | Stable under normal conditions. |

APPLICATIONS

Tert-butyl acetate (TBAC) is an oxygenated solvent used alone or in blends for coatings, industrial cleaning and surface treatment applications. It is a substitute for HAP (Hazardous Air Pollutant) solvents, VOCs (volatile organic compounds: acetaldehyde, benzene, 1,3-butadiene, ethylbenzene, formaldehyde, toluene, xylenes, and particulate organic matter), chlorinated solvents and other ozone depleters as well as esters and ethers in a short supply. It is also used as a process solvent for chemical reactions and polymerization. TBAC is a tert-butyl protecting group for organic synthesis. It undergoes Claisen condensation reaction for C-C bond formation. It is used as a component of aroma. It is used as an intermediate to manufacture pharmaceuticals, synthetic flavorings 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. | 1213 |

OTHER INFORMATION

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

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 conducive 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), (CH₃OH) and acetic acid (CH₃COOH) 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 [(CH₃)₂C=O], ethyl acetate (CH₃COOCH₂CH₃), methyl ethyl ketone, acetonitrile, N,N-dimethylformamide and diemthyl sulfoxide. Nonpolar solvents, like carbon tetrachloride (CCl₄), benzene (C₆H₆), and diethyl ether (CH₃CH₂OCH₂CH₃), 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 [(CH₃)₂C=O] and ethyl acetate (CH₃COOCH₂CH₃). Polar protic solvents are useful in S_N1 reaction, while polar aprotic solvents are S_N2 reaction.