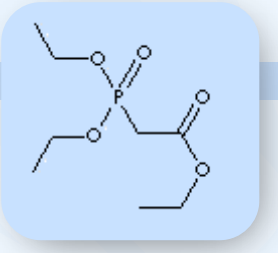
TRIETHYL PHOSPHONOACETATE

SYNONYMS

(Ethoxycarbonylmethyl)diethoxyphospshine oxide; (Diethylphosphono)acetic acid ethyl ester; Diethyl carbethoxymethylphosphonate; Diethyl carboethoxymethylphosphonate; Phosphono acetic acid triethyl ester; Diethyl ethoxycarbonylmethanephosphonate; Diethyl phosphonoacetic acid ethyl ester; Ethyl (diethoxyphosphinyl)acetate; Ethyl (diethoxyphosphoryl)acetate; Ethyl (diethylphosphono)acetate; Ethyl diethoxyphosphoryl acetate; Triethyl phosphonoacetate; Triethyl phosphonoethanoate; (Diethoxyphosphinyl)acetic acid ethyl ester; 2-(Diethoxyphosphinyl) acetic acid ethyl ester; Diethylphosphono acetic acid ethyl ester;



PRODUCT IDENTIFICATION

CAS RN	867-13-0; 874204-68-9
EINECS RN	212-757-6
FORMULA	$(C_2H_5O)_2P(O)CH_2COOC_2H_5$
MOL WEIGHT	224.19

PHYSICAL AND CHEMICAL PROPERTIES

PHYSICAL STATE	colorless to light yellow liquid
MELTING POINT	
BOILING POINT	260 - 262 C
DENSITY	1.13
SOLUBILITY IN WATER	
pH	
VAPOR DENSITY	
REFRACTIVE INDEX	1.4300 - 1.4320
FLASH POINT	> 112 C

APPLICATION

Horner-Wadsworth-Emmons Reaction:
The HWE reaction is the reaction of a carbonyl compound with an a-metalated phosphonate to give an alkene. The reaction is usually used when the nucleophilic carbon bears a strong anion stabilizing group (CO_2Me, COMe, COH, CN, SO_2R, SOR, vinyl, phenyl). Like the analogous Wittig reagents, the metalated phosphonates tend to give trans olefins if the substituents on phosphorus are simple alkoxy groups, and if lithium or sodium counterions are used. They can become cis-selective if non-coordinating cations (e.g., K^+ - 18-crown-6) or electron withdrawing substituents on the phosphonate ester groups are used (e.g. CF3CH2O- or ArO). In the absence of a carbanion-stabilizing group the elimination reaction to form the double bond becomes very slow. Apparently the transition state for the syn-elimination resembles the carbanion formed by cleavage of the P-C bond: Metalated phosphonates are substantially more reactive than analogous Wittig reagents, and will react with ketones as well as aldehydes. This can be predicted from the much higher basicity of phosphonates. Stabilized Wittig reagents react only with aldehydes. (source: http://www.chem.wisc.edu/)

These contain groups that can stabilise the negative charge from the carbanion-like carbon, for example Ph3P=CH-COOR, Ph3P=CH-Ph. These are less reactive than simple ylides, and so they usually fail to react with ketones, necessitating the use of the Horner-Wadsworth-Emmons reaction as an alternative. They can be prepared from the phosphonium salts using weaker bases than butyllithium such as alkoxides and (in some cases) sodium hydroxide. They usually give rise to an E-alkene product when they react, rather than the more usual Z-alkene. (source: http://www.spiritus-temporis.com/)

Horner-Wadsworth-Emmons Reagents

STABILITY AND REACTIVITY

TRIETHYL PHOSPHONOACETATE

STABILITY	Stable under normal conditions.
CONDITIONS OF INSTABILITY	Incompatible materials, ignition sources, excess heat, strong oxidants.
INCOMPATIBLE MATERIALS	Strong oxidizing agents.
DECOMPOSITION PRODUCTS	Phosphine, carbon monoxide, carbon dioxide, phosphorus oxides.
POLYMERIZATION	Will not occur

SAFETY

HAZARD NOTES	Irritating to eyes, respiratory system and skin.
EYE	Cause eye irritation.
SKIN	Cause skin irritation.
INGESTION	May cause gastrointestinal irritation with nausea, vomiting and diarrhea.
INHALATION	Cause respiratory tract irritation.
CHRONIC	
NFPA RATING	Health: , Flammability: , Reactivity:

SALES SPECIFICATION

APPEARANCE	colorless to light yellow liquid
ASSAY	98.0% min
COLOR	50 max (APHA)
REFRACTIVE INDEX	1.4300 - 1.4320

TRANSPORT & REGULATORY INFORMATION

UN NO.	
HAZARD CLASS	
PACKING GROUP	
HAZARD SYMBOL	XI
RISK PHRASES	36/37/38
SAFETY PHRASES	26-37/39

PACKING

PRICE