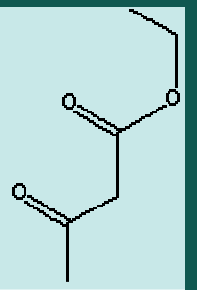
ETHYL ACETOACETATE



PRODUCT IDENTIFICATION	
CAS NO.	141-97-9
EINECS NO.	205-516-1
FORMULA	$CH_3COCH_2COOC_2H_5$
MOL WT.	130.14
H.S. CODE	2918.30
DERIVATION	
TOXICITY	Oral rat LD50: 3980 mg/kg
SYNONYMS	Acetoacetic ester; EAA; Ethyl beta-ketobutyrate; Acetoacetic ester, diacetic ether; Ethyl 3-oxobutanoate; Ethyl acetoacetate; Ethyl acetylacetate;3-Oxobutanoic acid ethyl ester; Ethyl 3-ketobutyrate; Ethyl acetylacetate; Ethyl acetonecarboxylate; Ethylacetoacetat (German); Acetoacetato de metilo (Spanish); Acétoacétate de méthyle (French);
CLASSIFICATION	ACETOACETIC ACID DERIVATIVES /

PHYSICAL AND CHEMICAL PROPERTIES	
PHYSICAL STATE	clear liquid,fruity odor
MELTING POINT	-40 C
BOILING POINT	181 C
SPECIFIC GRAVITY	1.03
SOLUBILITY IN WATER	Slightly soluble (completely soluble in alcohol and ether)
pH	4.0
VAPOR DENSITY	
AUTOIGNITION	295 C
NFPA RATINGS	Health: 2; Flammability: 2; Reactivity: 0
REFRACTIVE INDEX	1.419
FLASH POINT	70 C
STABILITY	Stable under ordinary conditions

GENERAL DESCRIPTION & APPLICATIONS

Diketene derivatives (mainly acetoacetic acid derivatives and heterocycle compounds) have versatile applications including making agrochemicals, dyes, pigments, pharmaceuticals including vitamins, and stabilizers for PVC and polyester. Acetoacetic acid and its esters contain active methylene groups which have relatively acidic alpha-protons due to H atoms adjacent to two carbonyl groups. The reactivity of its methylene group provide the sequence of reactions of alkylation, hydrolysis of the esters and decarboxylation resulting in substituted ketones. The methylene group can be reacted to form amino-carbonyl compounds. Acetoacetates are important aliphatic parts adjoining azo dyes and pigments. Acetoacetic acid is unstable and decompose to acetone and carbon dioxide at room temperature.

Ethyl acetoacetate has a reactive hydrogen atom on the carbon alpha to both carbonyl groups. It undergoes Knoevenagel condensation reaction as a reactant to forms a large class of target products including amino acids, drugs (analgesics, antibiotics, antimalarial agents, antipyrene andaminopyrene), and vitamin B1. It is also involved in the production of colorants, lacquers, perfumes, and plastics. Alone, it is used as a flavoring agent and a solvent. Knoevenagel condensation is a nucleophilic addition of a reactive hydrogen atom at 1,3-diketone compounds to a carbonyl group, followed by an dehydration reaction. 1,3-Diketone compounds (beta-ketones) include malonic acid, diethyl malonate, Meldrum's acid, and

acetoacetic acid derivatives.	
SALES SPECIFICATION	
APPEARANCE	clear liquid
PURITY	99.0% min
SPECIFIC GRAVITY	1.03
COLOR, APHA	10 max
TRANSPORTATION	
PACKING	200kgs in drum
HAZARD CLASS	3 (Packing Group: III)
UN NO.	1993
OTHER INFORMATION	
Hazard Symbols: XI, Risk Phrases: 36/37/38, Safety Phrases: 50A-9-16-26-33-37/39	