



>>Entry Name: Ethyl acetoacetate, 8CI

ENTRY UNDER REVIEW

Synonym(s): Ethyl 3-oxobutanoate, 9CI. Acetoacetic ester. Ethyl 3-hydroxy-2-butenate. FEMA 2415

Related CAS Registry Numbers(s): 19232-39-4 22157-27-3 22157-28-4 57031-90-0 57592-45-7

$\text{H}_3\text{CCOCH}_2\text{COOEt} \rightleftharpoons \text{H}_3\text{CC}(\text{OH})=\text{CHCOOEt}$

Molecular Formula:  $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

General Statement: Equilibrium mixt. consists of approx. 92.3% oxo and 7.7% enol forms at r.t. Both forms have been obt. at low temps.

Source/Synthesis: Obt. by condensation of ethyl acetate with sodium

Biological Source: Present in strawberry, yellow passion fruit juice and coffee

Use/Importance: Synthetic reagent of great utility and historical importance. Acetals with ethylene and propylene glycols are used in perfumery. Used as EtOH soln. as a metal indicator in titrimetry with EDTA of Fe(III) (pH range 1-2; colour change red-violet → pale yellow). Flavouring agent

Physical Description: Liq. with characteristic agreeable/irritant odour

pKa Value:  $\text{p}K_{\text{a}}$  11.8 (50% dioxan)  $\text{p}K_{\text{a}}$  10.68 (25°)

Hazard & Toxicity: Flammable, fl. p. 57/68/84°, autoignition temp. 295°

>>Variant: Oxo-form

CAS Registry Number: 141-97-9

Molecular Formula:  $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Liq.

Boiling Point:  $\text{Bp}_{14}$  74°.  $\text{Bp}_1$  28.5°

Solubility: Misc. most org. solvents, sol. dil. alkalis, pptd. with  $\text{CO}_2$ , spar. sol.  $\text{H}_2\text{O}$

Density:  $d^{20}_4$  1.0282

Refractive Index:  $n^{20}_D$  1.4190

Hazard & Toxicity: Mod. toxic. Eye and skin irritant.  $\text{LD}_{50}$  (rat, orl) 3980 mg/kg

Aldrich: 24070-2

Fluka: 420

Sigma: A8646

>>Derivative: Semicarbazone

CAS Registry Number: 5982-65-0

Physical Description: Needles ( $\text{Et}_2\text{O}$ )

Melting Point: Mp 129 dec.°

Solubility: Sol. hot  $\text{H}_2\text{O}$

>>Derivative: Phenylhydrazone

CAS Registry Number: 6078-46-2

Physical Description: Needles

Melting Point: Mp 50°

Solubility: Sol. EtOH

Other Data: Oxidised by air

>>Variant: Enol-form

CAS Registry Number: 1522-29-8

Molecular Formula:  $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

Physical Description: Oil

Refractive Index:  $n^{20}_D$  1.4480