



>>Entry Name: 3-Oxobutanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): Acetoacetic acid. Acetonecarboxylic acid. Acetylacetic acid. Diacetic acid

CAS Registry Number: 541-50-4

$\text{H}_3\text{CCOCH}_2\text{COOH} \leftrightarrow \text{H}_3\text{CC}(\text{OH})=\text{CHCOOH}$

Molecular Formula: $\text{C}_4\text{H}_6\text{O}_3$

Molecular Weight: 102.09

Accurate Mass: 102.031695

Percentage Composition: C 47.06%; H 5.92%; O 47.02%

Physical Description: Syrup or cryst.

Melting Point: Mp 36-37°

Boiling Point: Bp 100° dec.

Solubility: Misc. H_2O

pKa Value: $\text{p}K_{\text{a}1}$ 3.6 (25°)

Other Data: Strong but unstable acid. On warming loses $\text{CO}_2 \rightarrow \text{Me}_2\text{CO}$

>>Derivative: Li salt

CAS Registry Number: 3483-11-2

Physical Description: Cryst. ($\text{MeOH/Et}_2\text{O}$)

Aldrich: 23383-8

Fluka: 478

Sigma: A8509

>>Derivative: Me ester

Synonym(s): Methyl acetoacetate

CAS Registry Number: 105-45-3

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_3$

Molecular Weight: 116.116

Accurate Mass: 116.047345

Percentage Composition: C 51.72%; H 6.94%; O 41.34%

Physical Description: Oil

Boiling Point: Bp₂₀ 169-170°

Solubility: Misc. H_2O

pKa Value: $\text{p}K_{\text{a}1}$ 10.72 (21°)

Other Data: *Cis*- and *trans*-enol forms detected spectroscopically

Hazard & Toxicity: Fl. p. 67/77/82°, autoignition temp. 280°. Eye and skin irritant. LD₅₀ (rat, orl) 3228 mg/kg

Aldrich: M2640-2

Fluka: 500

Sigma: M4376

>>Derivative: Et ester

>>Derivative: Propyl ester

Synonym(s): Propyl acetoacetate

CAS Registry Number: 1779-60-8

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_3$

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Physical Description: Oil

Boiling Point: Bp₆ 66-69°