>>**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
H_3CCOCH_2COOH << >> $H_3CC(OH)=CHCOOH$

Molecular Formula: $C_4H_6O_3$
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: pK_{a1} 3.6 (25°)
Other Data: Strong but unstable acid. On warming loses $CO_2 \rightarrow Me_2CO$

>>**Derivative:** Li salt

CAS Registry Number: 3483-11-2
Physical Description: Cryst. ($MeOH/Et_2O$)
Aldrich: 23383-8
Fluka: 478
Sigma: A8509

>>**Derivative:** Me ester
Synonym(s): Methyl acetoacetate

CAS Registry Number: 105-45-3
Molecular Formula: $C_5H_8O_3$
Molecular Weight: 116.116
Accurate Mass: 116.047345
Percentage Composition: C 51.72%; H 6.94%; O 41.34%
Physical Description: Oil
Boiling Point: Bp_{20} 169-170°
Solubility: Misc. H_2O
pKa Value: pK_{a1} 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. LD_{50} (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: $C_7H_{12}O_3$
Molecular Weight: 144.17
Accurate Mass: 144.078645
Percentage Composition: C 58.32%; H 8.39%; O 33.29%
Physical Description: Oil
Boiling Point: Bp_6 66-69°