



Fluka: 485
Rare Chemicals Library: S61512-9

>>**Derivative:** Butyl ester
Synonym(s): Butyl acetoacetate. FEMA 2176

CAS Registry Number: 591-60-6
Molecular Formula: C₈H₁₄O₃
Molecular Weight: 158.197
Accurate Mass: 158.094295
Percentage Composition: C 60.74%; H 8.92%; O 30.34%
Physical Description: Oil
Boiling Point: Bp₆ 83-85°. Bp₁₆ 100-103°
Density: d²⁵ 0.98
Refractive Index: n_D²⁰ 1.4245

>>**Derivative:** *tert*-Butyl ester
Synonym(s): *tert*-Butyl acetoacetate

CAS Registry Number: 1694-31-1
Molecular Formula: C₈H₁₄O₃
Molecular Weight: 158.197
Accurate Mass: 158.094295
Percentage Composition: C 60.74%; H 8.92%; O 30.34%
Use/Importance: Reagent for acyloin and αβ-unsatd. ketone synth.
Physical Description: Oil
Boiling Point: Bp₂₀ 85°
Aldrich: B8860-8
Fluka: 450

>>**Derivative:** 2-Propenyl ester
Synonym(s): 2-Propenyl 3-oxobutanoate. Allyl acetoacetate

CAS Registry Number: 1118-84-9
Molecular Formula: C₇H₁₀O₃
Molecular Weight: 142.154
Accurate Mass: 142.062995
Percentage Composition: C 59.14%; H 7.09%; O 33.76%
Physical Description: Liq.
Boiling Point: Bp₂₁ 93°

>>**Derivative:** Benzyl ester
Synonym(s): Benzyl acetoacetate

CAS Registry Number: 5396-89-4
Molecular Formula: C₁₁H₁₂O₃
Molecular Weight: 192.214
Accurate Mass: 192.078645
Percentage Composition: C 68.74%; H 6.29%; O 24.97%
Physical Description: Oil
Boiling Point: Bp₂ 118-122°. Bp₁₀ 156-159°
Refractive Index: n_D²⁰ 1.5120
Aldrich: 29589-2
Fluka: 445

>>**Derivative:** Ph ester
Synonym(s): Phenyl acetoacetate

CAS Registry Number: 6864-62-6
Molecular Formula: C₁₀H₁₀O₃
Molecular Weight: 178.187
Accurate Mass: 178.062995
Percentage Composition: C 67.41%; H 5.66%; O 26.94%
Physical Description: Oil
Boiling Point: Bp_{0.2} 80-82°