



CAS Registry Number: 2343-88-6
Molecular Formula: C₄H₅FO₂
Molecular Weight: 104.081
Accurate Mass: 104.027358
Percentage Composition: C 46.16%; H 4.84%; F 18.25%; O 30.74%
Use/Importance: Acetoacetylating agent for alcohols and amines
Boiling Point: Bp 132-134°
Other Data: Dec. slowly at r.t., can be stored at 0°

>>**Derivative:** Chloride
Synonym(s): Acetoacetyl chloride

Molecular Formula: C₄H₅ClO₂
Molecular Weight: 120.535
Accurate Mass: 119.997807
Percentage Composition: C 39.86%; H 4.18%; Cl 29.41%; O 26.55%
Physical Description: Liq.
Melting Point: Mp -51°
Other Data: Unstable above -20°

>>**Derivative:** Amide
Synonym(s): 3-Oxobutanamide, 9Cl. Acetoacetamide

CAS Registry Number: 5977-14-0
Molecular Formula: C₄H₇NO₂
Molecular Weight: 101.105
Accurate Mass: 101.047679
Percentage Composition: C 47.52%; H 6.98%; N 13.85%; O 31.65%
Use/Importance: Reagent for synth. of heterocycles
Physical Description: Cryst. (Me₂CO/petrol)
Melting Point: Mp 54°
Solubility: Sol. H₂O, EtOH, AcOH
Other Data: Dec. on attempted dist.
Aldrich: 32881-2
Fluka: 405

>>**Derivative:** Methylamide
Synonym(s): *N*-Methyl-3-oxobutanamide, 9Cl

CAS Registry Number: 20306-75-6
Molecular Formula: C₅H₉NO₂
Molecular Weight: 115.132
Accurate Mass: 115.063329
Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%
Physical Description: Cryst. (Et₂O)
Melting Point: Mp 47°
Boiling Point: Bp_{0.8} 100-102°

>>**Derivative:** Dimethylamide
Synonym(s): *N,N*-Dimethylacetoacetamide. DMAA

CAS Registry Number: 2044-64-6
Molecular Formula: C₆H₁₁NO₂
Molecular Weight: 129.158
Accurate Mass: 129.078979
Percentage Composition: C 55.80%; H 8.58%; N 10.84%; O 24.77%
Boiling Point: Bp₁₀ 109°
Refractive Index: n_D²⁰ 1.4710
Other Data: Light sensitive
Aldrich: 40705-4
Sigma: D9546