



>>Entry Name: 2-Chloro-3-oxobutanoic acid

Synonym(s): 2-Chloroacetoacetic acid

CAS Registry Number: 5819-34-1

Related CAS Registry Numbers(s): 119878-78-3

H3CCOCHClCOOH

Molecular Formula: C4H5ClO3

Molecular Weight: 136.534

Accurate Mass: 135.992722

Percentage Composition: C 35.19%; H 3.69%; Cl 25.97%; O 35.15%

>>Variant: (±)-form

Molecular Formula: C4H5ClO3

Molecular Weight: 136.534

Accurate Mass: 135.992722

Percentage Composition: C 35.19%; H 3.69%; Cl 25.97%; O 35.15%

>>Derivative: Me ester

CAS Registry Number: 4755-81-1

Molecular Formula: C5H7ClO3

Molecular Weight: 150.561

Accurate Mass: 150.008372

Percentage Composition: C 39.89%; H 4.69%; Cl 23.55%; O 31.88%

Physical Description: Liq.

Melting Point: Mp -33°

Boiling Point: Bp 137°

Density: d_4^{20} 1.24

Refractive Index: n_D^{20} 1.4460

Aldrich: 18391-1

>>Derivative: Et ester

CAS Registry Number: 609-15-4

Molecular Formula: C6H9ClO3

Molecular Weight: 164.588

Accurate Mass: 164.024022

Percentage Composition: C 43.79%; H 5.51%; Cl 21.54%; O 29.16%

Physical Description: Liq.

Boiling Point: Bp 193° dec., Bp₃₀ 105-110°

Solubility: Sol. EtOH, Et₂O etc.; spar. sol. H₂O

Density: d_4^{20} 1.19

Refractive Index: n_D^{20} 1.4410

Aldrich: E1690-2

Fluka: 22811

>>Derivative: Amide

Synonym(s): 2-Chloroacetoacetamide

CAS Registry Number: 67271-66-3

Molecular Formula: C4H6ClNO2

Molecular Weight: 135.55

Accurate Mass: 135.008706

Percentage Composition: C 35.44%; H 4.46%; Cl 26.15%; N 10.33%; O 23.61%

Physical Description: Solid by subl.

Melting Point: Mp 76-77°