



>>Entry Name: 4-Chloro-3-oxobutanoic acid

Synonym(s): 4-Chloro-3-hydroxy-2-butenic acid. 4-Chloroacetoacetic acid

CAS Registry Number: 27807-84-7

ClCH2COCH2COOH<<>>ClCH2C(OH)=CHCOOH

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%

Physical Description: Cryst. (C₆H₆/petrol or by subl.)

Melting Point: Mp 67-69°

Boiling Point: Subl._{0.001} 55-58°

>>Derivative: Me ester

CAS Registry Number: 32807-28-6

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%

Use/Importance: Pharmaceutical intermed.

Physical Description: Liq.

Boiling Point: Bp₁₁ 96-97°. Bp₄ 85°

Density: d₄²⁰ 1.31

Refractive Index: n_D²⁰ 1.4560

Hazard & Toxicity: Lachrymator. Irritant. Highly toxic by inhalation or skin absorption

Aldrich: 24586-0

Fluka: 22818

>>Derivative: Et ester

CAS Registry Number: 638-07-3

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%

Use/Importance: Shows fungicidal props.

Physical Description: Liq.

Melting Point: Fp -8°

Boiling Point: Bp 220° dec.. Bp₁₁ 101°

Solubility: Sol. org. solvs.; prac. insol. H₂O

Density: d₄²⁰ 1.22

Other Data: Turns yellow on standing. Irritant to skin and mucous membranes

Hazard & Toxicity: Irritant. Highly toxic by inhalation or skin absorption

Aldrich: 18076-9

Fluka: 22813

>>Derivative: Chloride

CAS Registry Number: 41295-64-1

Molecular Formula: C₄H₄Cl₂O₂

Molecular Weight: 154.98

Accurate Mass: 153.958834

Percentage Composition: C 31.00%; H 2.60%; Cl 45.75%; O 20.65%

Use/Importance: Pharmaceutical intermed.

>>Variant: (E)-Enol-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%