



>>Entry Name: 2-Chloro-2-methylpropanoic acid, 9CI

Synonym(s): 2-Chloroisobutyric acid

CAS Registry Number: 594-58-1

(H₃C)₂CClCOOH

Molecular Formula: C₄H₇ClO₂

Molecular Weight: 122.551

Accurate Mass: 122.013457

Percentage Composition: C 39.20%; H 5.76%; Cl 28.93%; O 26.11%

Physical Description: Liq.

Melting Point: Mp 31°

Boiling Point: Bp₅₀ 118°. Bp₁₂ 80-82°

Solubility: Sol. H₂O

pKa Value: pK_a 2.98 (18°)

>>Derivative: Me ester

CAS Registry Number: 22421-97-2

Molecular Formula: C₅H₉ClO₂

Molecular Weight: 136.578

Accurate Mass: 136.029107

Percentage Composition: C 43.97%; H 6.64%; Cl 25.96%; O 23.43%

Boiling Point: Bp 133-135°

>>Derivative: Chloride

CAS Registry Number: 13222-26-9

Molecular Formula: C₄H₆Cl₂O

Molecular Weight: 140.996

Accurate Mass: 139.979569

Percentage Composition: C 34.07%; H 4.29%; Cl 50.29%; O 11.35%

Boiling Point: Bp 126-127° (113-114°)

>>Derivative: Nitrile

Synonym(s): 2-Chloro-2-cyanopropane

CAS Registry Number: 3331-60-0

Molecular Formula: C₄H₆ClN

Molecular Weight: 103.551

Accurate Mass: 103.018876

Percentage Composition: C 46.40%; H 5.84%; Cl 34.24%; N 13.53%

Boiling Point: Bp₆ 52°

References:

Michael, A., *Ber.*, 1901, **34**, 4054, (*synth*)

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Chrzaszczewska, A. *et al.*, *CA*, 1928, **22**, 2146, (*synth*)

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Ogata, Y. *et al.*, *J.O.C.*, 1975, **40**, 2960, (*synth*)

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