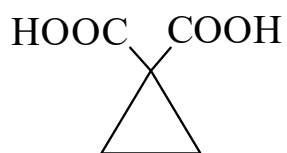




>>Entry Name: 1,1-Cyclopropanedicarboxylic acid, 9CI

Synonym(s): Ethylenemalonic acid. Vinaconic acid



CAS Registry Number: 598-10-7

Molecular Formula: C₅H₆O₄

Molecular Weight: 130.1

Accurate Mass: 130.02661

Percentage Composition: C 46.16%; H 4.65%; O 49.19%

Physical Description: Prisms or needles (CHCl₃), prisms + 1H₂O (H₂O)

Melting Point: Mp 140°

Solubility: Sol. H₂O, org. solvs.

pKa Value: pK_{a1} 1.68; pK_{a2} 7.22 (25°)

Aldrich: 34341-2

Fluka: 29915

>>Derivative: Di-Me ester

CAS Registry Number: 6914-71-2

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Boiling Point: Bp₇₆₄ 198°

Aldrich: 41278-3

>>Derivative: Mono-Et ester

CAS Registry Number: 3697-66-3

Molecular Formula: C₇H₁₀O₄

Molecular Weight: 158.154

Accurate Mass: 158.05791

Percentage Composition: C 53.16%; H 6.37%; O 40.47%

Physical Description: Yellowish oil

>>Derivative: Di-Et ester

CAS Registry Number: 1559-02-0

Molecular Formula: C₉H₁₄O₄

Molecular Weight: 186.207

Accurate Mass: 186.08921

Percentage Composition: C 58.05%; H 7.58%; O 34.37%

Physical Description: Liq.

Boiling Point: Bp₂₂ 115°

Aldrich: 14771-0

Fluka: 29920

>>Derivative: Monoamide

CAS Registry Number: 6914-74-5

Molecular Formula: C₅H₇NO₃

Molecular Weight: 129.115

Accurate Mass: 129.042594

Percentage Composition: C 46.51%; H 5.46%; N 10.85%; O 37.17%

Physical Description: Cryst.

Melting Point: Mp 195°

Aldrich: 43951-7

Other: Oakwood 1454