



>>Entry Name: 2,2-Dimethylbutanedioic acid

Synonym(s): 2,2-Dimethylsuccinic acid

CAS Registry Number: 597-43-3

HOCCC(CH3)2CH2COOH

Molecular Formula: C₆H₁₀O₄

Molecular Weight: 146.143

Accurate Mass: 146.05791

Percentage Composition: C 49.31%; H 6.90%; O 43.79%

Melting Point: Mp 141°

pKa Value: pK_a 4.09 (25°)

Aldrich: D18600-7

Fluka: 39660

Sigma: D3394

>>Derivative: 1-Me ester

CAS Registry Number: 32980-26-0

Molecular Formula: C₇H₁₂O₄

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Melting Point: Mp 41°

Boiling Point: Bp₁₄ 141°

pKa Value: pK_a 4.59

>>Derivative: 4-Me ester

CAS Registry Number: 54043-71-9

Molecular Formula: C₇H₁₂O₄

Molecular Weight: 160.169

Accurate Mass: 160.07356

Percentage Composition: C 52.49%; H 7.55%; O 39.96%

Melting Point: Mp 52°

pKa Value: pK_a 4.64

>>Derivative: Di-Me ester

CAS Registry Number: 49827-44-3

Molecular Formula: C₈H₁₄O₄

Molecular Weight: 174.196

Accurate Mass: 174.08921

Percentage Composition: C 55.16%; H 8.10%; O 36.74%

Boiling Point: Bp 201-202°. Bp₁₇ 91-92°

>>Derivative: Dichloride

CAS Registry Number: 66734-50-7

Molecular Formula: C₆H₈Cl₂O₂

Molecular Weight: 183.033

Accurate Mass: 181.990134

Percentage Composition: C 39.37%; H 4.41%; Cl 38.74%; O 17.48%

Boiling Point: Bp 200-202° dec.

>>Derivative: 1-Nitrile, 4-Et ester

Synonym(s): Ethyl 3-cyano-3-methylbutanoate, 9CI

CAS Registry Number: 100568-19-2

Molecular Formula: C₈H₁₃NO₂

Molecular Weight: 155.196

Accurate Mass: 155.094629

Percentage Composition: C 61.91%; H 8.44%; N 9.03%; O 20.62%

Physical Description: Liq.

Boiling Point: Bp_{0.6} 68-70°