



>>Entry Name: Dimethylpropanedioic acid, 9CI

Synonym(s): Dimethylmalonic acid, 8CI

CAS Registry Number: 595-46-0

$(\text{H}_3\text{C})_2\text{C}(\text{COOH})_2$

Molecular Formula: $\text{C}_5\text{H}_8\text{O}_4$

Molecular Weight: 132.116

Accurate Mass: 132.04226

Percentage Composition: C 45.46%; H 6.10%; O 48.44%

Physical Description: Prisms (C_6H_6 /petrol)

Melting Point: Mp 192-193°

Solubility: Sol. hot H_2O

pKa Value: $\text{p}K_{\text{a}1}$ 3.03; $\text{p}K_{\text{a}2}$ 5.73 (25°)

Other Data: Subl. >130° with part. dec.

Aldrich: D16800-9

Fluka: 40760

>>Derivative: Mono-Me ester

CAS Registry Number: 13051-21-3

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_4$

Molecular Weight: 146.143

Accurate Mass: 146.05791

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

Melting Point: Mp 35-38°

>>Derivative: Di-Me ester

CAS Registry Number: 6065-54-9

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_4$

Molecular Weight: 160.169

Accurate Mass: 160.07356

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

Physical Description: Liq.

Boiling Point: Bp 177-178°. Bp₂₂ 71°

>>Derivative: Di-Et ester

CAS Registry Number: 1619-62-1

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_4$

Molecular Weight: 188.223

Accurate Mass: 188.10486

Percentage Composition: C 57.43%; H 8.57%; O 34.00%

Physical Description: Liq.

Boiling Point: Bp 196-198°. Bp₁₇ 83-84°

Aldrich: 14390-1

>>Derivative: Dichloride

CAS Registry Number: 5659-93-8

Molecular Formula: $\text{C}_5\text{H}_6\text{Cl}_2\text{O}_2$

Molecular Weight: 169.007

Accurate Mass: 167.974484

Percentage Composition: C 35.53%; H 3.58%; Cl 41.95%; O 18.93%

Physical Description: Liq.

Boiling Point: Bp 165°

Aldrich: 39190-5

Fluka: 40758