



>>Entry Name: **3-Oxopentanedioic acid**, 9CI

Synonym(s): 3-Oxoglutaric acid, 8CI. Acetone-1,3-dicarboxylic acid

CAS Registry Number: 542-05-2

HOOCCH₂COCH₂COOH

Molecular Formula: C₅H₆O₅

Molecular Weight: 146.099

Accurate Mass: 146.021525

Percentage Composition: C 41.11%; H 4.14%; O 54.76%

Use/Importance: Intermed. in Robinson tropinone synth. and other heterocyclic syntheses. Used in 1,3-annulation of imines

Physical Description: Needles (EtOAc)

Melting Point: Mp 135 dec.°

Solubility: Sol. H₂O, EtOH; insol. CHCl₃, C₆H₆

Other Data: Decarboxylated by hot H₂O, acids or alkalis

Aldrich: 16511-5

Fluka: 600

Sigma: K1376

>>Derivative: Di-Me ester

CAS Registry Number: 1830-54-2

Molecular Formula: C₇H₁₀O₅

Molecular Weight: 174.153

Accurate Mass: 174.052825

Percentage Composition: C 48.28%; H 5.79%; O 45.93%

Boiling Point: Bp₂₅ 150°

Aldrich: D13800-2

Fluka: 640

Sigma: D3387

>>Derivative: Mono-Et ester

Molecular Formula: C₇H₁₀O₅

Molecular Weight: 174.153

Accurate Mass: 174.052825

Percentage Composition: C 48.28%; H 5.79%; O 45.93%

Melting Point: Mp 86°

>>Derivative: Di-Et ester

CAS Registry Number: 105-50-0

Molecular Formula: C₉H₁₄O₅

Molecular Weight: 202.207

Accurate Mass: 202.084125

Percentage Composition: C 53.46%; H 6.98%; O 39.56%

Boiling Point: Bp₁₂ 138°

Aldrich: 16512-3

Fluka: 630

>>Derivative: Di-Et ester, semicarbazone

Melting Point: Mp 94-95°

>>Derivative: Di-*tert*-butyl ester

CAS Registry Number: 28009-80-5

Molecular Formula: C₁₃H₂₂O₅

Molecular Weight: 258.314

Accurate Mass: 258.146725

Percentage Composition: C 60.45%; H 8.58%; O 30.97%

Physical Description: Cryst. (hexane/EtOAc)

Melting Point: Mp 60-61°

Aldrich: 27081-4

Fluka: 635