



>>Entry Name: 3-Oxohexanedioic acid, 9CI

Synonym(s): 3-Oxoadipic acid

CAS Registry Number: 689-31-6

HOOCCH₂COCH₂CH₂COOH

Molecular Formula: C₆H₈O₅

Molecular Weight: 160.126

Accurate Mass: 160.037175

Percentage Composition: C 45.01%; H 5.04%; O 49.96%

Physical Description: Plates (Me₂CO/CHCl₃)

Melting Point: Mp 124-125 dec.°

Aldrich: 26834-8

Sigma: K0500

>>Derivative: Di-Me ester

CAS Registry Number: 5457-44-3

Molecular Formula: C₈H₁₂O₅

Molecular Weight: 188.18

Accurate Mass: 188.068475

Percentage Composition: C 51.06%; H 6.43%; O 42.51%

Boiling Point: Bp₁₈ 150°

Refractive Index: n_D²⁰ 1.4450

Aldrich: D16760-6

Fluka: 75808

>>Derivative: Di-Et ester

CAS Registry Number: 7149-59-9

Molecular Formula: C₁₀H₁₆O₅

Molecular Weight: 216.233

Accurate Mass: 216.099775

Percentage Composition: C 55.55%; H 7.46%; O 37.00%

Boiling Point: Bp_{0.35} 109-111°

Sigma: K2252

>>Derivative: 1-Mononitrile

Synonym(s): 5-Cyano-4-oxopentanoic acid

Molecular Formula: C₆H₇NO₃

Molecular Weight: 141.126

Accurate Mass: 141.042594

Percentage Composition: C 51.06%; H 5.00%; N 9.92%; O 34.01%

Physical Description: Cryst. (CHCl₃)

Melting Point: Mp 86-88°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1109C, (*nmr*)

Aldrich Library of Infrared Spectra, 3rd edn., 1981, 403E, (*ir*)

Eisner, U. *et al.*, *J.C.S.*, 1950, 2223, (*synth*)

Taylor, E.C. *et al.*, *Tetrahedron*, 1967, **23**, 897, (*synth, bibl*)