>>**Entry Name: 3-Oxohexanedioic acid,** 9Cl
Synonym(s): 3-Oxoadipic acid

CAS Registry Number: 689-31-6
$HOOCCH_2COCH_2CH_2COOH$

Molecular Formula: $C_6H_8O_5$
Molecular Weight: 160.126
Accurate Mass: 160.037175
Percentage Composition: C 45.01%; H 5.04%; O 49.96%
Physical Description: Plates ($Me_2CO/CHCl_3$)
Melting Point: Mp 124-125 dec.°

Aldrich: 26834-8
Sigma: K0500

>>**Derivative:** Di-Me ester

CAS Registry Number: 5457-44-3
Molecular Formula: $C_8H_{12}O_5$
Molecular Weight: 188.18
Accurate Mass: 188.068475
Percentage Composition: C 51.06%; H 6.43%; O 42.51%
Boiling Point: Bp_{18} 150°
Refractive Index: n_D^{20} 1.4450
Aldrich: D16760-6
Fluka: 75808

>>**Derivative:** Di-Et ester

CAS Registry Number: 7149-59-9
Molecular Formula: $C_{10}H_{16}O_5$
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: $C_6H_7NO_3$
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. ($CHCl_3$)
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)*