>>**Entry Name: 4,6-Dioxoheptanoic acid,** 9CI
Synonym(s): 5-Acetyl-4-oxopentanoic acid. Succinylacetone

CAS Registry Number: 51568-18-4
Related CAS Registry Numbers(s): 20754-03-4 135884-28-5
Type of Compound Code(s): VY0900
$H_3CCOCH_2COCH_2CH_2COOH$

Molecular Formula: $C_7H_{10}O_4$
Molecular Weight: 158.154
Accurate Mass: 158.05791
Percentage Composition: C 53.16%; H 6.37%; O 40.47%
General Statement: Enolised β-diketone
Biological Source: Constit. of various biol. fluids
Use/Importance: Precursor of tetrapyrroles
Biological Use/Importance: Tyrosine metabolite and 5-aminolevulinic acid dehydrase inhibitor. Immunosuppressant
Physical Description: Cryst. ($CHCl_3$/CCl_4)
Melting Point: Mp 67-69°

Aldrich: 28414-9
Sigma: D8645

>>**Derivative:** Me ester

CAS Registry Number: 80480-42-8
Molecular Formula: $C_8H_{12}O_4$
Molecular Weight: 172.18
Accurate Mass: 172.07356
Percentage Composition: C 55.81%; H 7.02%; O 37.17%
Physical Description: Oil
Boiling Point: $Bp_{0.05}$ 81-83°

>>**Derivative:** Et ester

CAS Registry Number: 20754-03-4
Molecular Formula: $C_9H_{14}O_4$
Molecular Weight: 186.207
Accurate Mass: 186.08921
Percentage Composition: C 58.05%; H 7.58%; O 34.37%
Physical Description: Oil
Boiling Point: Bp_{13} 140-141°. $Bp_{0.1}$ 91°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 824A, *(nmr)*
Pendarvis, R.O. *et al.*, *J.O.C.*, 1974, **39**, 2289-2291, *(synth)*
Tschudy, D.P. *et al.*, *J. Biol. Chem.*, 1981, **256**, 9915-9923, *(biochem)*
Battersby, A.R. *et al.*, *J.C.S. Perkin 1*, 1981, 2786-2799, *(Me ester, synth, props)*
Lindblad, B. *et al.*, *Biomed. Mass Spectrom.*, 1982, **9**, 419-424, *(ms, occur)*
Lash, T.D. *et al.*, *J.O.C.*, 1999, **64**, 478-487, *(Me ester)*