



>>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

H3CCOCH2COCH2CH2COOH

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: Bp₁₃ 140-141°. Bp_{0.1} 91°

References:

Aldrich Library of ^{13}C 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 I*, 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*)