



>>Entry Name: 4-Acetyl-5-oxohexanoic acid

Synonym(s): 4,4-Diacetylbutyric acid

CAS Registry Number: 54605-46-8

$(\text{H}_3\text{CCO})_2\text{CHCH}_2\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_8\text{H}_{12}\text{O}_4$

Molecular Weight: 172.18

Accurate Mass: 172.07356

Percentage Composition: C 55.81%; H 7.02%; O 37.17%

>>Derivative: Me ester

CAS Registry Number: 13984-53-7

Molecular Formula: $\text{C}_9\text{H}_{14}\text{O}_4$

Molecular Weight: 186.207

Accurate Mass: 186.08921

Percentage Composition: C 58.05%; H 7.58%; O 34.37%

Physical Description: Liq.

Boiling Point: Bp₂₄ 160-161°. Bp₅ 117-121°

Aldrich: 29617-1

>>Derivative: Et ester

CAS Registry Number: 2832-10-2

Molecular Formula: $\text{C}_{10}\text{H}_{16}\text{O}_4$

Molecular Weight: 200.234

Accurate Mass: 200.10486

Percentage Composition: C 59.98%; H 8.05%; O 31.96%

Physical Description: Liq.

Boiling Point: Bp₁₅ 154-155°. Bp_{0.8} 111-114°

Aldrich: 30160-4

>>Derivative: Et ester, dioxime

Molecular Formula: $\text{C}_{10}\text{H}_{18}\text{N}_2\text{O}_4$

Molecular Weight: 230.263

Accurate Mass: 230.126658

Percentage Composition: C 52.16%; H 7.88%; N 12.17%; O 27.79%

Physical Description: Prisms

Melting Point: Mp 108-110°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **1**, 1106B; 1106C, (*nmr*)

Johnson, A.W. *et al.*, *J.C.S.*, 1958, 4254, (*synth*)

Chong, R. *et al.*, *Aust. J. Chem.*, 1967, **20**, 123, (*synth, ir, pmr*)

Rapoport, H. *et al.*, *J.O.C.*, 1971, **36**, 853, (*synth, pmr*)