



>>Entry Name: 3-Oxoheptanoic acid, 9CI
Synonym(s): *n*-Valerylacetic acid. Pentanoylacetic acid

CAS Registry Number: 63563-21-3
H3C(CH2)3COCH2COOH

Molecular Formula: C7H12O3
Molecular Weight: 144.17
Accurate Mass: 144.078645
Percentage Composition: C 58.32%; H 8.39%; O 33.29%

>>Derivative: Me ester

CAS Registry Number: 39815-78-6
Molecular Formula: C8H14O3
Molecular Weight: 158.197
Accurate Mass: 158.094295
Percentage Composition: C 60.74%; H 8.92%; O 30.34%
Physical Description: Liq.
Boiling Point: Bp_{0.1} 54-55°
Density: d²⁵ 0.989
Refractive Index: n_D²⁵ 1.4315

>>Derivative: Et ester

CAS Registry Number: 7737-62-4
Molecular Formula: C9H16O3
Molecular Weight: 172.224
Accurate Mass: 172.109945
Percentage Composition: C 62.77%; H 9.36%; O 27.87%
Boiling Point: Bp₁₅ 111°

References:

Hauser, C.R. *et al.*, *J.A.C.S.*, 1946, **68**, 26
Matsura, S. *et al.*, *Yakugaku Zasshi*, 1951, **71**, 802
Mageswaran, S. *et al.*, *J.C.S. Perkin 1*, 1976, 884
Oikawa, Y. *et al.*, *J.O.C.*, 1978, **43**, 2087
Cadman, M.L.F. *et al.*, *J.C.S. Perkin 1*, 1995, 1397, (*Me ester, synth, pmr, ir*)