



>>Entry Name: 3-Oxohexanoic acid, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3-Oxocaproic acid. Butyrylacetic acid

CAS Registry Number: 4380-91-0

$\text{H}_3\text{CCH}_2\text{CH}_2\text{COCH}_2\text{COOH}$

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3$

Molecular Weight: 130.143

Accurate Mass: 130.062995

Percentage Composition: C 55.37%; H 7.74%; O 36.88%

>>Derivative: Me ester

CAS Registry Number: 30414-54-1

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_3$

Molecular Weight: 144.17

Accurate Mass: 144.078645

Percentage Composition: C 58.32%; H 8.39%; O 33.29%

Boiling Point: Bp_{14} 85°

>>Derivative: Et ester

Synonym(s): FEMA 3683

CAS Registry Number: 3249-68-1

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_3$

Molecular Weight: 158.197

Accurate Mass: 158.094295

Percentage Composition: C 60.74%; H 8.92%; O 30.34%

Physical Description: Liq. with a slightly fatty odour

Boiling Point: Bp_{20} 102-103°. $\text{Bp}_{0.5}$ 57-60°

Refractive Index: n_D^{20} 1.4362

Aldrich: E1580-9

Fluka: 20790

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 690A, (*ir*)

Aldrich Library of ^{13}C and ^1H FT NMR Spectra, 1992, **1**, 1104C, (*nmr*)

Kagan, H.B. *et al.*, *Bull. Soc. Chim. Fr.*, 1966, 1819, (*synth*)

Kaneda, A. *et al.*, *Bull. Chem. Soc. Jpn.*, 1967, **40**, 228, (*synth*)

Roth, M. *et al.*, *Helv. Chim. Acta*, 1971, **54**, 710, (*synth*)

Rathke, M.W. *et al.*, *Tet. Lett.*, 1971, 2953, (*synth*)

Couffignal, R. *et al.*, *J. Organomet. Chem.*, 1977, **127**, C65, (*synth*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, **2**, 261, (*Et ester*)

Cadman, M.L.F. *et al.*, *J.C.S. Perkin I*, 1995, 1397, (*Me ester, synth, ir, pmr*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1029, (*Et ester*)