



>>Entry Name: 3,3-Dimethyl-4-pentenoic acid

CAS Registry Number: 7796-73-8

$\text{H}_2\text{C}=\text{CHC}(\text{CH}_3)_2\text{CH}_2\text{COOH}$

Molecular Formula: $\text{C}_7\text{H}_{12}\text{O}_2$

Molecular Weight: 128.171

Accurate Mass: 128.08373

Percentage Composition: C 65.60%; H 9.44%; O 24.97%

Physical Description: Liq.

Boiling Point: Bp₄ 83-85°

>>Derivative: Me ester

CAS Registry Number: 63721-05-1

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_2$

Molecular Weight: 142.197

Accurate Mass: 142.09938

Percentage Composition: C 67.57%; H 9.92%; O 22.50%

Physical Description: Liq.

Boiling Point: Bp₃₃ 59°

Aldrich: 34724-8

>>Derivative: Et ester

CAS Registry Number: 7796-72-7

Molecular Formula: $\text{C}_9\text{H}_{16}\text{O}_2$

Molecular Weight: 156.224

Accurate Mass: 156.11503

Percentage Composition: C 69.19%; H 10.32%; O 20.48%

Physical Description: Liq.

Boiling Point: Bp₇₂ 94-98°. Bp_{0.1} 35-45°

>>Derivative: Chloride

CAS Registry Number: 88819-78-7

Molecular Formula: $\text{C}_7\text{H}_{11}\text{ClO}$

Molecular Weight: 146.616

Accurate Mass: 146.049842

Percentage Composition: C 57.35%; H 7.56%; Cl 24.18%; O 10.91%

Physical Description: Pale-yellow liq.

Boiling Point: Bp₄₅ 71-72°

References:

Aldrich Library of ¹³C and ¹H FT NMR Spectra, 1992, **1**, 984C, (nmr)

Jöger, V. *et al.*, *Tet. Lett.*, 1977, 2543, (synth)

Nakada, Y. *et al.*, *Bull. Chem. Soc. Jpn.*, 1979, **52**, 1511, (deriv, synth, ir, pmr)

Beckwith, A.F.J., *Aust. J. Chem.*, 1983, **36**, 545, (synth, pmr)

Kleschick, W.A. *et al.*, *J.O.C.*, 1986, **51**, 5429, (synth, ir, pmr)

Li, W. *et al.*, *J.O.C.*, 1995, **60**, 8155, (synth, pmr, cmr, ms)