



>>Entry Name: 4-Methyl-4-pentenoic acid

CAS Registry Number: 1001-75-8

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

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_2$

Molecular Weight: 114.144

Accurate Mass: 114.06808

Percentage Composition: C 63.14%; H 8.83%; O 28.03%

Boiling Point: $\text{Bp}_{0.85}$ 59-61°

>>Derivative: Et ester

CAS Registry Number: 4911-54-0

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%

Boiling Point: Bp_{57} 98-100°. Bp_{20} 85°

Aldrich: 33939-3

>>Derivative: Nitrile

Synonym(s): 4-Methyl-4-pentenitrile. 4-Cyano-2-methyl-1-butene

CAS Registry Number: 34998-36-2

Molecular Formula: $\text{C}_6\text{H}_9\text{N}$

Molecular Weight: 95.144

Accurate Mass: 95.073499

Percentage Composition: C 75.74%; H 9.53%; N 14.72%

Biological Source: Constit. of *Capparis flexuosa*

Boiling Point: Bp_{12} 50-51°

References:

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

Jones, D.T. *et al.*, *J.C.S.*, 1904, **85**, 1691, (synth)

Mori, K. *et al.*, *Agric. Biol. Chem.*, 1975, **39**, 1889, (synth, ir, pmr)

Grob, C.A. *et al.*, *Helv. Chim. Acta*, 1979, **62**, 1854-1865, (synth, nitrile)

Mazzocchi, P.H. *et al.*, *J.O.C.*, 1983, **48**, 2981, (synth, pmr)

Gramosa, N.V. *et al.*, *J. Essent. Oil Res.*, 1997, **9**, 709-712, (isol, nitrile)

Buffet, M.F. *et al.*, *J.C.S. Perkin 1*, 2000, 1815-1827, (synth, Et ester, ir, pmr, cmr)