



>>Entry Name: 4-Pentynoic acid, 9CI

CAS Registry Number: 6089-09-4

HC≡CCH₂CH₂COOH

Molecular Formula: C₅H₆O₂

Molecular Weight: 98.101

Accurate Mass: 98.03678

Percentage Composition: C 61.22%; H 6.16%; O 32.62%

Physical Description: Cryst.

Melting Point: Mp 57°

pKa Value: pK_a 4.2 (25°, 0.1M NaCl)

Aldrich: 23221-1

Fluka: 77055

>>Derivative: Me ester

CAS Registry Number: 21565-82-2

Molecular Formula: C₆H₈O₂

Molecular Weight: 112.128

Accurate Mass: 112.05243

Percentage Composition: C 64.27%; H 7.19%; O 28.54%

Boiling Point: Bp 143-144°. Bp₁₇₅ 101-102°

>>Derivative: *p*-Bromophenacyl ester

Physical Description: Long needles

Melting Point: Mp 103°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-1-butyne. 4-Pentynenitrile

CAS Registry Number: 19596-07-7

Molecular Formula: C₅H₅N

Molecular Weight: 79.101

Accurate Mass: 79.042199

Percentage Composition: C 75.92%; H 6.37%; N 17.71%

Boiling Point: Bp₁₂ 57-58°. Bp₁₀ 60°

Refractive Index: n_D²³ 1.4369

Rare Chemicals Library: S10095-1

References:

- Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **2**, 943C, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 525C, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1595C, (*ir*)
Colonge, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1954, 797, (*synth*)
Schulte, K.E. *et al.*, *Chem. Ber.*, 1954, **87**, 964, (*synth*)
Compagnon, P.L. *et al.*, *Bull. Soc. Chim. Fr.*, 1968, 2105, (*nitrile*)
Holland, B.C. *et al.*, *Synth. Commun.*, 1974, **4**, 203, (*synth, ir, pmr*)
Martel, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1978, 131, (*synth*)
Wulff, W.D. *et al.*, *J.A.C.S.*, 1988, **110**, 7419, (*synth, pmr*)
Messer, W.S. *et al.*, *J. Med. Chem.*, 1997, **40**, 1230-1246, (*nitrile, synth, pmr*)