



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

CAS Registry Number: 10602-00-3

Structure by analogy with 2-Ethynylbenzoic acid, [HXB04-K](#)

Molecular Formula: C₉H₆O₂

Molecular Weight: 146.145

Accurate Mass: 146.03678

Percentage Composition: C 73.97%; H 4.14%; O 21.90%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 224-225°

Other Data: Darkens rapidly on exp. to air

>>Derivative: Me ester

CAS Registry Number: 3034-86-4

Molecular Formula: C₁₀H₈O₂

Molecular Weight: 160.172

Accurate Mass: 160.05243

Percentage Composition: C 74.99%; H 5.03%; O 19.98%

Physical Description: Cryst.

Melting Point: Mp 92.5-93.5°

>>Derivative: Et ester

CAS Registry Number: 10602-03-6

Molecular Formula: C₁₁H₁₀O₂

Molecular Weight: 174.199

Accurate Mass: 174.06808

Percentage Composition: C 75.84%; H 5.79%; O 18.37%

Physical Description: Oil

>>Derivative: Chloride

CAS Registry Number: 62480-31-3

Molecular Formula: C₉H₅ClO

Molecular Weight: 164.591

Accurate Mass: 164.002892

Percentage Composition: C 65.68%; H 3.06%; Cl 21.54%; O 9.72%

Physical Description: Yellow cryst.

Melting Point: Mp 78-79°

>>Derivative: Nitrile

CAS Registry Number: 3032-96-0

Molecular Formula: C₉H₅N

Molecular Weight: 127.145

Accurate Mass: 127.042199

Percentage Composition: C 85.02%; H 3.96%; N 11.02%

Physical Description: Solid

Melting Point: Mp 156-157°

References:

Eaborn, C. *et al.*, *J.C.S.(C)*, 1967, 1364-1366, (*synth*)

Takashashi, S. *et al.*, *Synthesis*, 1980, 627-630, (*nitrile, synth, ir, pmr*)

Austin, W.B. *et al.*, *J.O.C.*, 1981, **46**, 2280-2286, (*synth, ir, pmr*)

Melissaris, A.P. *et al.*, *J.O.C.*, 1992, **57**, 6998-6999, (*synth, chloride, ir, pmr*)

Negishi, E. *et al.*, *J.O.C.*, 1997, **62**, 8957-8960, (*Me ester, synth, pmr, cmr*)

Okumura, K. *et al.*, *J. Med. Chem.*, 1998, **41**, 4036-4052, (*nitrile*)

Iijima, T. *et al.*, *Chem. Pharm. Bull.*, 1999, **47**, 388-404, (*Et ester, synth, pmr*)