



>>Entry Name: 3-Biphenylcarboxylic acid

Synonym(s): *m*-Phenylbenzoic acid

CAS Registry Number: 716-76-7

Molecular Formula: C₁₃H₁₀O₂

Molecular Weight: 198.221

Accurate Mass: 198.06808

Percentage Composition: C 78.77%; H 5.08%; O 16.14%

Physical Description: Leaflets (H₂O)

Melting Point: Mp 167-168°

pKa Value: pK_a 5.46 (25°, 5.29, 50% aq. EtOH)

>>Derivative: Me ester

CAS Registry Number: 16606-00-1

Molecular Formula: C₁₄H₁₂O₂

Molecular Weight: 212.248

Accurate Mass: 212.08373

Percentage Composition: C 79.23%; H 5.70%; O 15.08%

Melting Point: Mp 160-161°

>>Derivative: Et ester

CAS Registry Number: 19926-50-2

Molecular Formula: C₁₅H₁₄O₂

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Physical Description: Oil

>>Derivative: Nitrile

CAS Registry Number: 24973-50-0

Molecular Formula: C₁₃H₉N

Molecular Weight: 179.221

Accurate Mass: 179.073499

Percentage Composition: C 87.12%; H 5.06%; N 7.82%

Boiling Point: Bp 118-120°

References:

Woods, G.F. *et al.*, *J.A.C.S.*, 1949, **71**, 2028-2031, (*synth*)

Drapala, T. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1964, **38**, 1593-1599, (*uv*)

Kobayashi, M. *et al.*, *Org. Prep. Proced.*, 1969, **1**, 221-224, (*nitrile, synth*)

Van Meurs, F. *et al.*, *J. Organomet. Chem.*, 1977, **142**, 299-308, (*pKa*)

Blackburn, A.C. *et al.*, *Acta Cryst. C*, 1996, **52**, 2320-2323, (*synth, cryst struct*)

Matsuhira, A. *et al.*, *Chem. Pharm. Bull.*, 1997, **45**, 1870-1874, (*synth, pmr*)

Bumagin, N.A. *et al.*, *Tetrahedron*, 1997, **53**, 14437-14450, (*synth*)