



>>Entry Name: 4'-Fluoro-4-biphenylcarboxylic acid

Synonym(s): 4-(4-Fluorophenyl)benzoic acid

CAS Registry Number: 5731-10-2

Structure by analogy with 2'-Fluoro-2-biphenylcarboxylic acid, [BJW43-O](#)

Molecular Formula: C₁₃H₉FO₂

Molecular Weight: 216.211

Accurate Mass: 216.058658

Percentage Composition: C 72.22%; H 4.20%; F 8.79%; O 14.80%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 236-238°

pKa Value: pK_a 5.51 (20°, 50% 2-butoxyethanol aq.)

>>Derivative: Me ester

Molecular Formula: C₁₄H₁₁FO₂

Molecular Weight: 230.238

Accurate Mass: 230.074308

Percentage Composition: C 73.03%; H 4.82%; F 8.25%; O 13.90%

Physical Description: Plates (EtOH aq.)

Melting Point: Mp 98.5-99.5°

>>Derivative: Nitrile

Synonym(s): 4-Cyano-4'-fluorobiphenyl

CAS Registry Number: 10540-31-5

Molecular Formula: C₁₃H₈FN

Molecular Weight: 197.211

Accurate Mass: 197.064077

Percentage Composition: C 79.18%; H 4.09%; F 9.63%; N 7.10%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 116-117°

References:

Dewar, M.J.S. *et al.*, *J.A.C.S.*, 1966, **88**, 3318, (*synth, nmr*)

Byron, D.J. *et al.*, *J.C.S.(C)*, 1966, 831; 840, (*synth*)

Gleason, W.B. *et al.*, *Acta Cryst. C*, 1991, **47**, 2137, (*cryst struct, nitrile*)