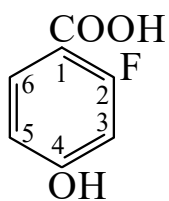




>>Entry Name: 2-Fluoro-4-hydroxybenzoic acid, 9CI



CAS Registry Number: 65145-13-3

Related CAS Registry Numbers(s): 321-24-4 394-42-3

Molecular Formula: C₇H₅FO₃

Molecular Weight: 156.113

Accurate Mass: 156.022273

Percentage Composition: C 53.86%; H 3.23%; F 12.17%; O 30.75%

Physical Description: Solid (EtOH aq.)

Melting Point: Mp 203-204°

pKa Value: pK_{a1} 3.8; pK_{a2} 8.5 (phenol)

>>Derivative: Nitrile

Synonym(s): 4-Hydroxy-2-fluorobenzonitrile. 4-Cyano-3-fluorophenol

CAS Registry Number: 82380-18-5

Molecular Formula: C₇H₄FNO

Molecular Weight: 137.113

Accurate Mass: 137.027692

Percentage Composition: C 61.32%; H 2.94%; F 13.86%; N 10.22%; O 11.67%

Physical Description: Solid (hexane/toluene)

Melting Point: Mp 117-118°

Aldrich: 41744-0

>>Derivative: 4-Me ether, nitrile

Synonym(s): 4-Methoxy-2-fluorobenzonitrile. 1-Cyano-2-fluoro-4-methoxybenzene

CAS Registry Number: 94610-82-9

Molecular Formula: C₈H₆FNO

Molecular Weight: 151.14

Accurate Mass: 151.043342

Percentage Composition: C 63.58%; H 4.00%; F 12.57%; N 9.27%; O 10.59%

Physical Description: Solid (MeOH)

Melting Point: Mp 59-60°

References:

Husain, M. *et al.*, *J. Biol. Chem.*, 1980, **255**, 4189, (*synth, uv*)

Kelly, S.M., *Helv. Chim. Acta*, 1984, **67**, 1572, (*nitrile*)