



>>Entry Name: 4-Amino-2-fluorophenol, 9CI

CAS Registry Number: 399-96-2

Molecular Formula: C₆H₆FNO

Molecular Weight: 127.118

Accurate Mass: 127.043342

Percentage Composition: C 56.69%; H 4.76%; F 14.95%; N 11.02%; O 12.59%

Physical Description: Pale brown prisms (C₆H₆)

Melting Point: Mp 162°

>>Derivative: N-Ac

CAS Registry Number: 2045-39-8

Molecular Formula: C₈H₈FNO₂

Molecular Weight: 169.155

Accurate Mass: 169.053907

Percentage Composition: C 56.80%; H 4.77%; F 11.23%; N 8.28%; O 18.92%

Physical Description: Cryst.

Melting Point: Mp 190-191°

>>Derivative: Me ether

Synonym(s): 3-Fluoro-4-methoxyaniline. 3-Fluoro-4-methoxybenzenamine, 9CI. 3-Fluoro-*p*-anisidine. 4-Amino-2-fluoroanisole

CAS Registry Number: 366-99-4

Molecular Formula: C₇H₈FNO

Molecular Weight: 141.145

Accurate Mass: 141.058992

Percentage Composition: C 59.57%; H 5.71%; F 13.46%; N 9.92%; O 11.34%

Physical Description: Cryst.

Melting Point: Mp 83°

Aldrich: 33487-1

>>Derivative: Me ether; hydrochloride

CAS Registry Number: 3803-20-1

Melting Point: Mp 180-200 dec.°

>>Derivative: Me ether, N-Ac

CAS Registry Number: 452-15-3

Molecular Formula: C₉H₁₀FNO₂

Molecular Weight: 183.182

Accurate Mass: 183.069557

Percentage Composition: C 59.01%; H 5.50%; F 10.37%; N 7.65%; O 17.47%

Melting Point: Mp 113°

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 518B, (*nmr*)
Schiemann, G. *et al.*, *Ber.*, 1933, **66**, 1179-1187, (*Me ether, synth*)
English, J. *et al.*, *J.A.C.S.*, 1940, **62**, 350-354, (*Me ether, synth*)
Berg, S.S. *et al.*, *J.C.S.*, 1949, 642-648, (*synth*)
Finger, G.C. *et al.*, *J.A.C.S.*, 1959, **81**, 94-101, (*Me ether, synth*)
Aymes, D.J. *et al.*, *Bull. Soc. Chim. Fr.*, 1980, 175-178, (*synth*)
Eur. Pat., 1988, 263 438; **109**, 110042s, (*synth*)
O'Neill, P.M. *et al.*, *J. Med. Chem.*, 1994, **37**, 1362-1370, (*deriv, synth, pmr, ir, ms*)