



>>Entry Name: 3-Fluorophenol, 9CI

CAS Registry Number: 372-20-3

Structure by analogy with 2-Fluorophenol, [DTN89-B](#)

Molecular Formula: C₆H₅FO

Molecular Weight: 112.103

Accurate Mass: 112.032443

Percentage Composition: C 64.29%; H 4.50%; F 16.95%; O 14.27%

Physical Description: Prisms or liq.

Melting Point: Mp 13.7°

Boiling Point: Bp 178°. Bp₇₀ 108°

Density: d^{15.2} 1.222

pKa Value: pK_a 9.21 (25°)

Aldrich: F1300-2

Fluka: 47271

Sigma: F3876

>>Derivative: Ac

CAS Registry Number: 701-83-7

Molecular Formula: C₈H₇FO₂

Molecular Weight: 154.14

Accurate Mass: 154.043008

Percentage Composition: C 62.34%; H 4.58%; F 12.33%; O 20.76%

Boiling Point: Bp₁₆ 77°

>>Derivative: Me ether

Synonym(s): 1-Fluoro-3-methoxybenzene. *m*-Fluoroanisole

CAS Registry Number: 456-49-5

Molecular Formula: C₇H₇FO

Molecular Weight: 126.13

Accurate Mass: 126.048093

Percentage Composition: C 66.66%; H 5.59%; F 15.06%; O 12.68%

Melting Point: Mp -35°

Boiling Point: Bp₇₄₃ 158°. Bp₁₅ 51°

Aldrich: 16231-0

Sigma: F8375

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-3-fluorobenzene. *m*-Fluorophenetole

CAS Registry Number: 458-03-7

Molecular Formula: C₈H₉FO

Molecular Weight: 140.157

Accurate Mass: 140.063743

Percentage Composition: C 68.56%; H 6.47%; F 13.56%; O 11.42%

Physical Description: Liq.

Melting Point: Mp -27.5°

Boiling Point: Bp 171.4°. Bp₁₅ 65.2°

References:

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Sadtler Standard Ultraviolet Spectra, 22141, (*uv*)

Finger, G.C. *et al.*, *J.A.C.S.*, 1959, **81**, 94, (*synth*)

McLafferty, F.W. *et al.*, *Arch. Mass Spectral Data*, 1970, **1**, 284, (*ms*)

Sterk, H. *et al.*, *Org. Magn. Reson.*, 1975, **7**, 275, (*nmr*)

Schaefer, T. *et al.*, *Can. J. Chem.*, 1989, **67**, 1027, (*pmr, F nmr, conformn, 3-fluoroanisole*)