



>>Entry Name: 4-Fluorophenol, 9CI

CAS Registry Number: 371-41-5

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

Molecular Formula: C<sub>6</sub>H<sub>5</sub>FO

Molecular Weight: 112.103

Accurate Mass: 112.032443

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

Melting Point: Mp 48°

Boiling Point: Bp 189°. Bp<sub>13</sub> 81.5°

pKa Value: pK<sub>a</sub> 9.91 (25°)

Hazard & Toxicity: Fl. p. 68°. LD<sub>50</sub> (mus, ipr) 312 mg/kg. Exp. carcinogenic and reprod. effects

Aldrich: F1320-7

Fluka: 47280

Sigma: F4001

>>Derivative: Ac

CAS Registry Number: 405-51-6

Molecular Formula: C<sub>8</sub>H<sub>7</sub>FO<sub>2</sub>

Molecular Weight: 154.14

Accurate Mass: 154.043008

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

Boiling Point: Bp<sub>16</sub> 85-87°. Bp<sub>4.5</sub> 54-55° (lit. gives a pressure range)

Aldrich: 46923-8

>>Derivative: Me ether

Synonym(s): 1-Fluoro-4-methoxybenzene. *p*-Fluoroanisole

CAS Registry Number: 459-60-9

Molecular Formula: C<sub>7</sub>H<sub>7</sub>FO

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 -45°

Boiling Point: Bp 157°. Bp<sub>21</sub> 60°

Aldrich: F460-2

Sigma: F8500

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-4-fluorobenzene. *p*-Fluorophenetole

CAS Registry Number: 459-26-7

Molecular Formula: C<sub>8</sub>H<sub>9</sub>FO

Molecular Weight: 140.157

Accurate Mass: 140.063743

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

Melting Point: Mp -8.5°

Boiling Point: Bp 173°. Bp<sub>18</sub> 71°

Rare Chemicals Library: S36209-3

#### References:

*Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 185B; 253A, (*nmr*)

*Aldrich Library of FT-IR Spectra, 1st edn.*, 1985, **1**, 1043A; 1078A

*Aldrich Library of FT-IR Spectra: Vapor Phase*, 1989, **3**, 971C; 1010D, (*ir*)

*Sadtler Standard C-13 NMR Spectra*, 4226, (*cmr*)

*Sadtler Standard Ultraviolet Spectra*, 21907, (*uv*)

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

Miyajima, G. *et al.*, *Org. Magn. Reson.*, 1972, **4**, 811, (*cmr*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, FKV000