



>>Entry Name: 5-Fluoro-2-nitrophenol

CAS Registry Number: 446-36-6

Structure by analogy with 2-Fluoro-4-nitrophenol, [DTN58-R](#)

Molecular Formula: C₆H₄FNO₃

Molecular Weight: 157.101

Accurate Mass: 157.017522

Percentage Composition: C 45.87%; H 2.57%; F 12.09%; N 8.92%; O 30.55%

Use/Importance: Has fungicidal props.

Physical Description: Yellow needles (petrol)

Melting Point: Mp 32°

pKa Value: pK_a 6.07 (25°)

Other Data: Steam-volatile

Hazard & Toxicity: Hazardous exothermic synth. on large scale

Aldrich: 23324-2

Fluka: 47178

Sigma: F6637

>>Derivative: O-Benzoyl

Molecular Formula: C₁₃H₈FNO₄

Molecular Weight: 261.209

Accurate Mass: 261.043737

Percentage Composition: C 59.78%; H 3.09%; F 7.27%; N 5.36%; O 24.50%

Melting Point: Mp 110-111°

>>Derivative: Me ether

Synonym(s): 4-Fluoro-2-methoxy-1-nitrobenzene. 5-Fluoro-2-nitroanisole

CAS Registry Number: 448-19-1

Molecular Formula: C₇H₆FNO₃

Molecular Weight: 171.128

Accurate Mass: 171.033172

Percentage Composition: C 49.13%; H 3.53%; F 11.10%; N 8.18%; O 28.05%

Physical Description: Cryst. (petrol)

Melting Point: Mp 52°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1362A, (*ir*)

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 734A, (*nmr*)

Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1208C, (*ir*)

Hodgson, H.H. *et al.*, *J.C.S.*, 1928, 1879, (*synth*)

Balasubramanian, A. *et al.*, *Can. J. Chem.*, 1966, **44**, 961, (*uv*)

Robinson, N., *Chem. Br.*, 1987, **23**, 837, (*haz*)