



>>Entry Name: 3-Ethylphenol, 9CI
Synonym(s): 1-Ethyl-3-hydroxybenzene

CAS Registry Number: 620-17-7
Extra CAS Registry Numbers(s): 25429-37-2
Structure by analogy with 2-Ethylphenol, [DTB48-G](#)

Molecular Formula: C₈H₁₀O
Molecular Weight: 122.166
Accurate Mass: 122.073165
Percentage Composition: C 78.65%; H 8.25%; O 13.10%
Melting Point: Mp -4°
Boiling Point: Bp₇₅₂ 214°
Density: d⁰ 1.025
pKa Value: pK_{a1} 10.07 (25°)

Aldrich: 28141-7
Fluka: 4690
Supelco: R42-5615

>>Derivative: Ac

CAS Registry Number: 3056-60-8
Molecular Formula: C₁₀H₁₂O₂
Molecular Weight: 164.204
Accurate Mass: 164.08373
Percentage Composition: C 73.15%; H 7.37%; O 19.49%
Melting Point: Mp 222-223°
Density: d⁰ 1.04

>>Derivative: Me ether

Synonym(s): 1-Ethyl-3-methoxybenzene. *m*-Ethylanisole

CAS Registry Number: 10568-38-4
Molecular Formula: C₉H₁₂O
Molecular Weight: 136.193
Accurate Mass: 136.088815
Percentage Composition: C 79.37%; H 8.88%; O 11.75%
Boiling Point: Bp₇₅₈ 196-197°. Bp₁₂ 77-78°
Rare Chemicals Library: S43133-8

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1073C, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1005C, (*ir*)
Aldrich Library of NMR Spectra, 2nd edn., 1983, **1**, 871B, (*nmr*)
Kenner, J. *et al.*, *J.C.S.*, 1935, 299, (*synth*)
Adv. Chem. Ser., 1955, **15**, 284, (*props*)
Brown, P., *Org. Mass Spectrom.*, 1969, **2**, 1317, (*ms*)
Fr. Pat., 1974, 2 202 068; *CA*, **82**, 111771, (*synth*)
Laurence, C. *et al.*, *Bull. Soc. Chim. Fr.*, 1977, 441, (*ir*)
Shapiro, B.L. *et al.*, *J. Phys. Chem. Ref. Data*, 1977, **6**, 919, (*nmr*)