



>>Entry Name: **2,3,5-Trimethylphenol**, 9Cl, 8Cl
Synonym(s): 6-Hydroxy-ψ-cumene. Iso-ψ-cumenol

CAS Registry Number: 697-82-5
Related CAS Registry Numbers(s): 56444-54-3
Extra CAS Registry Numbers(s): 26998-80-1

Molecular Formula: C₉H₁₂O
Molecular Weight: 136.193
Accurate Mass: 136.088815
Percentage Composition: C 79.37%; H 8.88%; O 11.75%
Physical Description: Cryst. (petrol)
Melting Point: Mp 95-96°
pKa Value: pK_{a1} 10.67 (25°)

Aldrich: T7860-3
Fluka: 92690
Supelco: 44-2286

>>Derivative: Phenylurethane

Physical Description: Needles (petrol)
Melting Point: Mp 174°

>>Derivative: Ac

Molecular Formula: C₁₁H₁₄O₂
Molecular Weight: 178.23
Accurate Mass: 178.09938
Percentage Composition: C 74.13%; H 7.92%; O 17.95%
Physical Description: Liq.
Boiling Point: Bp 241°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-2,3,5-trimethylbenzene. 2,3,5-Trimethylanisole

CAS Registry Number: 20469-61-8
Molecular Formula: C₁₀H₁₄O
Molecular Weight: 150.22
Accurate Mass: 150.104465
Percentage Composition: C 79.96%; H 9.39%; O 10.65%
Physical Description: Liq.
Boiling Point: Bp₇₅₅ 214-216°

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 282C, (nmr)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1093B, (ir)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1030A, (ir)
Wehrli, P.A. *et al.*, *J.O.C.*, 1972, **37**, 2340, (synth)