



>>Entry Name: 2,4,6-Trimethylphenol, 9CI
Synonym(s): Mesitol, 8CI. Hydroxymesitylene

CAS Registry Number: 527-60-6
Related CAS Registry Numbers(s): 51114-00-2 79719-34-9
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: Needles (EtOH)
Melting Point: Mp 69°
Boiling Point: Bp 220°
pKa Value: pK_a 9.98 (25°)
Other Data: Sublimes, steam-volatile

Aldrich: T7900-6
Fluka: 92710
Supelco: R42-8080

>>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 236°

>>Derivative: Phenylurethane

Melting Point: Mp 141-142°

>>Derivative: Me ether
Synonym(s): 2-Methoxy-1,3,5-trimethylbenzene. 2,4,6-Trimethylanisole. Methoxymesitylene

CAS Registry Number: 4028-66-4
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: Bp 200-203°

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1094B, (*ir*)
Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 284A, (*nmr*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1031A, (*ir*)
Eberson, L. *et al.*, *Acta Chem. Scand., Ser. B*, 1975, **29**, 168-171, (*synth*)
Wu, C. *et al.*, *J. Med. Chem.*, 1999, **42**, 4485-4499, (*Me ether, synth, pmr*)