



>>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: C<sub>9</sub>H<sub>12</sub>O  
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<sub>a1</sub> 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: C<sub>11</sub>H<sub>14</sub>O<sub>2</sub>  
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: C<sub>10</sub>H<sub>14</sub>O  
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<sub>755</sub> 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)