



>>Entry Name: 2,4,5-Trimethylphenol, 9CI, 8CI

Synonym(s): 5-Hydroxy- ξ -cumene. ψ -Cumenol. Pseudocumenol

CAS Registry Number: 496-78-6

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 70°

pKa Value: pK_a 9.96 (25°)

Rare Chemicals Library: S45878-3

>>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: Needles (petrol)

Melting Point: Mp 34-34.5°

Boiling Point: Bp 245-246°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-2,4,5-trimethylbenzene. 2,4,5-Trimethylanisole

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 213-214°

References:

Colonge, J. *et al.*, *Bull. Soc. Chim. Fr.*, 1962, 96, (*synth*)