



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

Synonym(s): 5-Hydroxy- $\xi$ -cumene.  $\psi$ -Cumenol. Pseudocumenol

CAS Registry Number: 496-78-6

Extra CAS Registry Numbers(s): 26998-80-1

Molecular Formula:  $C_9H_{12}O$

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 70°

pKa Value:  $pK_a$  9.96 (25°)

Rare Chemicals Library: S45878-3

>>Derivative: Ac

Molecular Formula:  $C_{11}H_{14}O_2$

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:  $C_{10}H_{14}O$

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 213-214°

#### References:

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