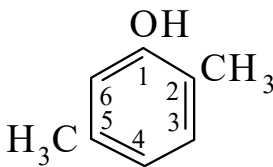




>>Entry Name: 2,5-Dimethylphenol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2,5-Xylenol, 8CI. *p*-2-Xylenol. Hydroxy-*p*-xylene. FEMA 3595



CAS Registry Number: 95-87-4

Extra CAS Registry Numbers(s): 1300-71-6 25155-23-1

Type of Compound Code(s): VG0010 WE9999 WI4000 WI4400

Molecular Formula: C₈H₁₀O

Molecular Weight: 122.166

Accurate Mass: 122.073165

Percentage Composition: C 78.65%; H 8.25%; O 13.10%

Biological Source: Isol. from Siberian conifer

Physical Description: Cryst. (EtOH)

Melting Point: Mp 71-73°

Boiling Point: Bp 210°. Bp₁₀ 89.3°

pKa Value: pK_a 10.41 (25°)

Hazard & Toxicity: LD₅₀ (rat, orl) 444 mg/kg

Aldrich: W35950-5

Fluka: 41330

Supelco: 44-2322

>>Derivative: Ac

CAS Registry Number: 877-48-5

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Physical Description: Oil

Boiling Point: Bp 237°

>>Derivative: 4-Nitrobenzoyl

CAS Registry Number: 135838-96-9

Physical Description: Cryst.

Melting Point: Mp 88°

>>Derivative: Me ether

Synonym(s): 2-Methoxy-1,4-dimethylbenzene, 9CI. 2,5-Dimethylanisole

CAS Registry Number: 1706-11-2

Molecular Formula: C₉H₁₂O

Molecular Weight: 136.193

Accurate Mass: 136.088815

Percentage Composition: C 79.37%; H 8.88%; O 11.75%

Physical Description: Liq.

Boiling Point: Bp 194°

Aldrich: 13748-0

Sigma: D3271

>>Derivative: Et ether

Synonym(s): 2-Ethoxy-1,4-dimethylbenzene, 9CI. 2,5-Dimethylphenetole

CAS Registry Number: 61808-03-5

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 199°