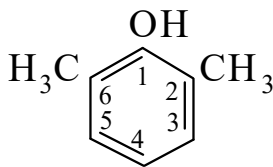




>>Entry Name: 2,6-Dimethylphenol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2,6-Xylenol, 8CI. *m*-2-Xylenol. 2-Hydroxy-*m*-xylene. 1,3,2-Xylenol. FEMA 3249



CAS Registry Number: 576-26-1

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

Type of Compound Code(s): PS8300 VG0010 WI4400 WI4000 WE9999 PS7700 PA2750

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 a Siberian conifer. Manuf. by vapour-phase alkylation of phenol with methanol

Use/Importance: Used as 0.1% soln. in glac. AcOH for extraction-photometric detn. of NO₃⁽⁻⁾ ($\lambda_{\max}$ 432 nm, ϵ 7900, toluene). Monomer for engineering plastic poly(phenylene oxide)

Physical Description: Leaflets or flat needles

Melting Point: Mp 49°

Boiling Point: Bp 203°

Solubility: Sol. EtOH, AcOH; mod. sol. H₂O

pKa Value: pK_a 10.62 (25°)

Other Data: Undergoes condensation polym. by oxidative coupling to give poly(phenylene oxide)

Hazard & Toxicity: Eye irritant. LD₅₀ (rat, orl) 296 mg/kg

Aldrich: D17500-5

Fluka: 41350

Sigma: D4261

Supelco: R42-8058

>>Derivative: Ac

CAS Registry Number: 876-98-2

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 215-216°. Bp_{0.3} 60°

>>Derivative: 4-Nitrobenzoyl

Physical Description: Cryst.

Melting Point: Mp 99°

>>Derivative: Me ether

Synonym(s): 2-Methoxy-1,3-dimethylbenzene. 2,6-Dimethylanisole

CAS Registry Number: 1004-66-6

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 182-183°. Bp₂₀ 79°

Aldrich: D14640-4