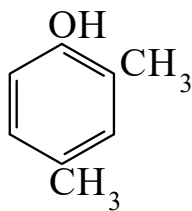




>>Entry Name: 2,4-Dimethylphenol

ENTRY UNDER REVIEW

Synonym(s): 2,4-Xylenol, 8Cl. *m*-4-Xylenol. 4-Hydroxy-*m*-xylene



CAS Registry Number: 105-67-9

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

Type of Compound Code(s): PS8300 PA2700

Molecular Formula: C₈H₁₀O

Molecular Weight: 122.166

Accurate Mass: 122.073165

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

Use/Importance: Used as 2.5% Me₂CO soln. for photometric detn. of NO₃⁽⁻⁾ (λ_{max} 455 nm)

Physical Description: Needles (EtOH aq. or C₆H₆)

Melting Point: Mp 27-28°

Boiling Point: Bp 210°. Bp₁₄ 97-98°

Solubility: Sol. Me₂CO, EtOH; mod. sol. H₂O

pKa Value: pK_a 10.6 (25°)

Hazard & Toxicity: LD₅₀ (rat, orl) 3200 mg/kg; LD₅₀ (rat, skn) 1040 mg/kg

Aldrich: 38374-0

Fluka: 41310

Supelco: R42-8054

>>Derivative: Ac

CAS Registry Number: 877-53-2

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: Bp₁₃ 107.5-108.5°

>>Derivative: Benzoyl

CAS Registry Number: 76048-43-6

Molecular Formula: C₁₅H₁₄O₂

Molecular Weight: 226.274

Accurate Mass: 226.09938

Percentage Composition: C 79.62%; H 6.24%; O 14.14%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 37-38°

Boiling Point: Bp₁₅ 110.5-111°

>>Derivative: Me ether

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

CAS Registry Number: 6738-23-4

Molecular Formula: C₉H₁₂O

Molecular Weight: 136.193

Accurate Mass: 136.088815

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

Physical Description: Oil

Boiling Point: Bp₁₃ 73-75°

Aldrich: 13747-2