



>>Entry Name: 3,4-Dimethylphenol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 3,4-Xylenol, 8CI. 4-Hydroxy-*o*-xylene. 1,2,4-Xylenol. *asym-o*-Xylenol. FEMA 3596

CAS Registry Number: 95-65-8

Related CAS Registry Numbers(s): 22618-23-1

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

Type of Compound Code(s): PA2700 WI5000 PS8300 WI4400 WE9999

Structure by analogy with 2,3-Dimethylphenol, [DZZ59-Q](#)

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 or 5% soln. in EtOH for photometric detn. of NO₃^m

Physical Description: Cryst. (H₂O)

Melting Point: Mp 62-64°

Boiling Point: Bp 227°

Solubility: Sol. EtOH; mod. sol. H₂O

pKa Value: pK_{a1} 10.36 (25°)

Hazard & Toxicity: LD₅₀ (rbt, orl) 800 mg/kg

Aldrich: D17540-4

Fluka: 41361

Supelco: R42-8062

>>Derivative: Ac

CAS Registry Number: 22618-23-1

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 220°. Bp₈₀ 140°

>>Derivative: Benzoyl

CAS Registry Number: 3845-63-4

Molecular Formula: C₁₅H₁₄O₂

Molecular Weight: 226.274

Accurate Mass: 226.09938

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

Melting Point: Mp 55-57°

>>Derivative: 4-Nitrobenzoyl

Physical Description: Cryst.

Melting Point: Mp 128°

>>Derivative: Me ether

Synonym(s): 4-Methoxy-1,2-dimethylbenzene, 9CI. 3,4-Dimethylanisole

CAS Registry Number: 4685-47-6

Molecular Formula: C₉H₁₂O

Molecular Weight: 136.193

Accurate Mass: 136.088815

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

Physical Description: Oil

Boiling Point: Bp 204-205°. Bp₁₇ 96-97°

Aldrich: 13749-9