



>>Entry Name: 3,5-Dimethylphenol

Synonym(s): 3,5-Xylenol, 8Cl. *m*-5-Xylenol. 5-Hydroxy-*m*-xylene

CAS Registry Number: 108-68-9

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

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%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 61 subl.° (68°)

Boiling Point: Bp 219.5°. Bp₁₀ 102.3°

pKa Value: p*K*_{a1} 10.19 (25°)

Hazard & Toxicity: Severe eye irritant. LD₅₀ (rat, orl) 608 mg/kg

Aldrich: D17570-6

Fluka: 41380

Rare Chemicals Library: S44941-5

Supelco: R42-8064

>>Derivative: Ac

CAS Registry Number: 877-82-7

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: Bp₁₁ 120°

Rare Chemicals Library: S3486-0

>>Derivative: 3,5-Dinitrobenzoyl

CAS Registry Number: 83612-63-9

Physical Description: Cryst. (EtOH)

Melting Point: Mp 195.4°

>>Derivative: Me ether

Synonym(s): 1-Methoxy-3,5-dimethylbenzene, 9Cl. 3,5-Dimethylanisole

CAS Registry Number: 874-63-5

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 193°

Aldrich: D14660-9

>>Derivative: Et ether

Synonym(s): 1-Ethoxy-3,5-dimethylbenzene, 9Cl. 3,5-Dimethylphenetole

CAS Registry Number: 18102-49-3

Molecular Formula: C₁₀H₁₄O

Molecular Weight: 150.22

Accurate Mass: 150.104465

Percentage Composition: C 79.96%; H 9.39%; O 10.65%

Physical Description: Oil

Boiling Point: Bp 208°

Rare Chemicals Library: S79826-6