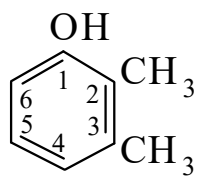




>>Entry Name: **2,3-Dimethylphenol**

Synonym(s): *o*-3-Xylenol. 3-Hydroxy-*o*-xylene. 1,2,3-Xylenol. 2,3-Xylenol. *vic-o*-Xylenol



CAS Registry Number: 526-75-0

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

Type of Compound Code(s): VG0010

Molecular Formula: C₈H₁₀O

Molecular Weight: 122.166

Accurate Mass: 122.073165

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

Biological Source: Constit. of *Angelica sinensis* and *Valerianella locusta*. Occurs in the defensive secretions of neotropical opilionids

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 75°

Boiling Point: Bp 218°. Bp₂₀ 120°

pKa Value: pK_a 10.54 (25°)

Refractive Index: n_D²⁰ 1.5420

Aldrich: D17400-9

Fluka: 41300

Supelco: 44-2292

>>Derivative: Ac

CAS Registry Number: 22618-22-0

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 226-228°. Bp₁₄ 107°. Bp₈ 104°

>>Derivative: Benzoyl

CAS Registry Number: 5554-27-8

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: Me ether

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

CAS Registry Number: 2944-49-2

Molecular Formula: C₉H₁₂O

Molecular Weight: 136.193

Accurate Mass: 136.088815

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

Physical Description: Cryst.

Melting Point: Mp 29°

Boiling Point: Bp 199°. Bp₁₅ 110°

Aldrich: 13746-4

Fluka: 39552