



>>Entry Name: 1,3-Benzenediol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Resorcinol, 8CI. 1,3-Dihydroxybenzene. Astriderm. Resorcin. Rezacuid. FEMA 3589

CAS Registry Number: 108-46-3

Extra CAS Registry Numbers(s): 12385-08-9

Molecular Formula: C₆H₆O₂

Molecular Weight: 110.112

Accurate Mass: 110.03678

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Use/Importance: Keratolytic, antiseptic. Used as 5% EtOH soln. for photometric detn. of Co, Zn, NO₂⁽⁻⁾, NO₃⁽⁻⁾. Used in manuf. of resorcinol-formaldehyde resins

Physical Description: Platelets (EtOH)

Melting Point: Mp 111°

Boiling Point: Bp 280°

Solubility: Sol. Et₂O, H₂O, EtOH, C₆H₆; sl. sol. CHCl₃

pKa Value: pK_{a1} 9.3; pK_{a2} 11.06 (20°)

Calculated Log P Data: Log P 0.81 (calc)

Hazard & Toxicity: Fl. p. 127°, autoignition temp. 608°. Skin and eye irritant. Possible skin sensitiser. Can cause restlessness, methaemoglobinaemia, convulsions and other systemic effects by skin absorption and ingestion. LD₅₀ (rat, orl) 301 mg/kg. OES: long-term 10 ppm; short-term 20 ppm

Aldrich: W35890-8

Fluka: 83602

Sigma: R5645

>>Derivative: Mono-Ac

Synonym(s): 3-Acetoxyphenol. **Resorcinol monoacetate**, USAN. Euresol

CAS Registry Number: 102-29-4

Molecular Formula: C₈H₈O₃

Molecular Weight: 152.149

Accurate Mass: 152.047345

Percentage Composition: C 63.15%; H 5.30%; O 31.55%

Use/Importance: Antiseborrheic, keratolytic agent

Physical Description: Oil

Boiling Point: Bp 283°

Calculated Log P Data: Log P 1 (calc)

Other Data: Component of Sulforcin

Hazard & Toxicity: Fl. p. >66°

Aldrich: R85-6

>>Derivative: Di-Ac

CAS Registry Number: 108-58-7

Molecular Formula: C₁₀H₁₀O₄

Molecular Weight: 194.187

Accurate Mass: 194.05791

Percentage Composition: C 61.85%; H 5.19%; O 32.96%

Physical Description: Liq.

Boiling Point: Bp 278°

Density: d²⁰ 1.178

Refractive Index: n_D²⁰ 1.5030

Hazard & Toxicity: Severe eye irritant

Aldrich: 27627-8