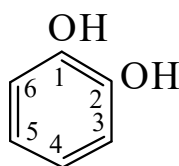




>>Entry Name: **1,2-Benzenediol**, 9CI

Synonym(s): Pyrocatechol, 8CI. **Catechol**‡. 1,2-Dihydroxybenzene. **Catechin (obsol.)**‡



CAS Registry Number: 120-80-9

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%

Biological Source: Isol. from various plant sources and by hydrol. of tannins

Use/Importance: Used as 5% aq. soln. for photometric detn. of Nb, Os, Ta, Ti, W; complexing agent of some metals (e.g. Al, Ti) (anionic complexes associated with basic dyes)

Biological Use/Importance: Antiseptic agent

Physical Description: Needles (H₂O)

Melting Point: Mp 105°

Boiling Point: Bp 240°

Solubility: Sol. H₂O, EtOH, Et₂O, C₆H₆, CHCl₃, Py

pKa Value: pK_{a1} 9.23; pK_{a2} 13 (25°)

Calculated Log P Data: Log P 0.88 (calc)

Other Data: Sublimes. Steam-volatile

Hazard & Toxicity: Explodes on contact with conc. HNO₃. Fl. p. 126/127°. Skin, eye and respiratory tract irritant. Prolonged or repeated exp. can also cause dermatitis. Cocarcinogen in exp. skin-painting studies. LD₅₀ (rat, orl) 260 mg/kg. LD₅₀ (rbt, skn) 800 mg/kg. Exp. reprod. effects. OES: long-term 5 ppm

Aldrich: 43074-9

Fluka: 15890

Sigma: C9510

>>Derivative: *O*-β-D-Glucopyranoside

CAS Registry Number: 2400-71-7

Molecular Formula: C₁₂H₁₆O₇

Molecular Weight: 272.254

Accurate Mass: 272.089605

Percentage Composition: C 52.94%; H 5.92%; O 41.14%

Biological Source: Isol. from leaves of *Gaultheria ovatifolia*, also in *Gaultheria humifusa*

Physical Description: Amorph. yellowish powder

Melting Point: Mp 130-140°

Optical Rotation: [α]_D²² -79 (c, 0.3 in EtOH)

>>Derivative: Di-*O*-β-D-glucopyranoside

Molecular Formula: C₁₈H₂₆O₁₂

Molecular Weight: 434.396

Accurate Mass: 434.14243

Percentage Composition: C 49.77%; H 6.03%; O 44.20%

Biological Source: Constit. of *Alangium premnifolium*

Physical Description: Needles (MeOH)

Melting Point: Mp 232-234°

Optical Rotation: [α]_D²⁸ -52.5 (c, 1 in H₂O)

UV: [neutral] λ_{max} 214 (log ε 3.85); 270 (log ε 3.11) (MeOH)