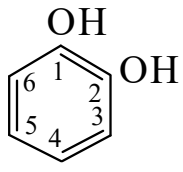
>>**Entry Name: 1,2-Benzenediol,** 9CI
Synonym(s): Pyrocatechol, 8CI. **Catechol‡.** 1,2-Dihydroxybenzene. **Catechin (obsol.)‡**



CAS Registry Number: 120-80-9
Extra CAS Registry Numbers(s): 12385-08-9

Molecular Formula: $C_6H_6O_2$
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 (H_2O)
Melting Point: Mp 105°
Boiling Point: Bp 240°
Solubility: Sol. H_2O, EtOH, Et_2O, C_6H_6, $CHCl_3$, 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. HNO_3. Fl. p. 126/127°. Skin, eye and respiratory tract irritant. Prolonged or repeated exp. can also cause dermatitis. Cocarcinogen in exp. skin-painting studies. LD_{50} (rat, orl) 260 mg/kg. LD_{50} (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: $C_{12}H_{16}O_7$
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: $[\alpha]_D^{22}$ –79 (c, 0.3 in EtOH)

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

Molecular Formula: $C_{18}H_{26}O_{12}$
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: $[\alpha]_D^{28}$ –52.5 (c, 1 in H_2O)
UV: [neutral] λ_{max} 214 (log ε 3.85); 270 (log ε 3.11) (MeOH)