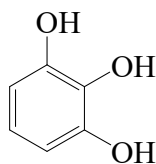




>>Entry Name: 1,2,3-Benzenetriol, 9CI

ENTRY UNDER REVIEW

Synonym(s): Pyrogallol, 8CI. 1,2,3-Trihydroxybenzene. Pyrogallic acid



CAS Registry Number: 87-66-1

Molecular Formula: C₆H₆O₃

Molecular Weight: 126.112

Accurate Mass: 126.031695

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Widespread in plants. Obt. comly. by decarboxylation of gallic acid (from galls)

Use/Importance: Reducing agent used in gas analysis, as photographic developer, etc. Used as 5% aq. soln. for gravimetric detn. of Sb, Bi, Mo, Ta, Th; photometric detn. of Ta. Polym. inhibitor for acrylic monomers. Has found use in adhesive applications

Biological Use/Importance: Formerly used topically for psoriasis and parasitic skin diseases

Physical Description: Plates or needles

Melting Point: Mp 133-134°

Boiling Point: Bp 309°. Bp₁₂ 171.5°

Solubility: V. sol. H₂O, EtOH, Et₂O; sl. sol. CHCl₃, C₆H₆; BERDY SOL: Sol. H₂O, MeOH, Et₂O, EtOH; poorly sol. C₆H₆, CHCl₃

pKa Value: pK_{a1} 9.28; pK_{a2} 11.34 (20°, μ = 0.1)

UV: [neutral] λ_{max} 244 (); 267 (); 275 () (MeOH) (Berdy)

Other Data: Bitter taste. Readily absorbs O₂

Hazard & Toxicity: Stains skin and hair black. Skin and eye irritant. Skin absorption can cause methaemoglobinaemia, haemolysis and kidney damage. LD₅₀ (mus, orl) 300 mg/kg. Exp. reprod. and tetraogenic effects

Aldrich: 14795-8

Fluka: 83130

Sigma: P2923

>>Derivative: 1-Ac

Synonym(s): Eugallol

CAS Registry Number: 1330-51-4

Molecular Formula: C₈H₈O₄

Molecular Weight: 168.149

Accurate Mass: 168.04226

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Use/Importance: Antipsoriatic

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 87-90°

>>Derivative: Tri-Ac

Synonym(s): Acetpyrogall. Lenigallol

CAS Registry Number: 525-52-0

Molecular Formula: C₁₂H₁₂O₆

Molecular Weight: 252.223

Accurate Mass: 252.06339

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Melting Point: Mp 165°

>>Derivative: Tribenzoyl

Molecular Formula: C₂₇H₁₈O₆

Molecular Weight: 438.436

Accurate Mass: 438.11034

Percentage Composition: C 73.97%; H 4.14%; O 21.90%

Physical Description: Prisms (EtOH)

Melting Point: Mp 89-90°