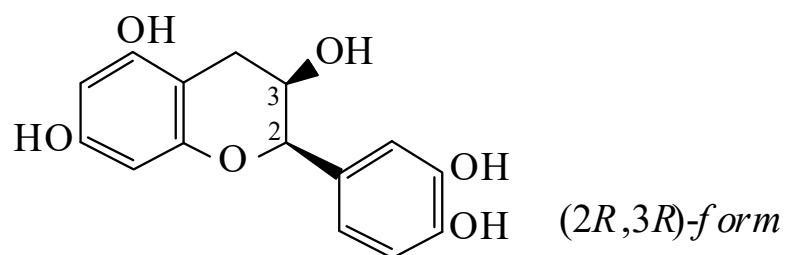




>>Entry Name: 3,3',4',5,7-Pentahydroxyflavan

ENTRY UNDER REVIEW

Synonym(s): 2-(3,4-Dihydroxyphenyl)-3,4-dihydro-2*H*-1-benzopyran-3,5,7-triol, 9Cl. 3',4',5,7-Tetrahydroxyflavanol



CAS Registry Number: 13392-26-2

Related CAS Registry Numbers(s): 72690-97-2 88191-48-4 88191-49-5 90276-13-4 99367-40-5

Molecular Formula: C₁₅H₁₄O₆

Molecular Weight: 290.272

Accurate Mass: 290.07904

Percentage Composition: C 62.07%; H 4.86%; O 33.07%

>>Variant: (2*R*,3*R*)-form

Synonym(s): (–)-*cis*-form. **Epicatechin**. Epicatechol. Teacatechin I. Acacatechin. Kakaol. Colatein

CAS Registry Number: 490-46-0

Extra CAS Registry Numbers(s): 321-01-7

Molecular Formula: C₁₅H₁₄O₆

Molecular Weight: 290.272

Accurate Mass: 290.07904

Percentage Composition: C 62.07%; H 4.86%; O 33.07%

Biological Source: Widespread

Biological Use/Importance: Antiinflammatory agent. Shows hepatotropic activity

Physical Description: Cryst.

Melting Point: Mp 242°

Optical Rotation: [α]_D –68 (EtOH)

Calculated Log P Data: Log P 0.38 (uncertain value) (calc)

UV: [neutral] λ_{max} 281 () (MeOH) (Berdy)

Aldrich: 85523-5

Fluka: 45300

Sigma: E1753

>>Derivative: 5-*O*-β-D-Xylopyranoside

Synonym(s): Epicatechin 5-xyloside

Molecular Formula: C₂₀H₂₂O₁₀

Molecular Weight: 422.388

Accurate Mass: 422.1213

Percentage Composition: C 56.87%; H 5.25%; O 37.88%

Biological Source: Constit. of *Brosimopsis acutifolium*

Physical Description: Amorph. powder

Optical Rotation: [α]_D –55 (c, 0.3 in MeOH)

>>Derivative: 3-*O*-β-D-Allopyranoside

Synonym(s): Epicatechin 3-alloside

CAS Registry Number: 98819-14-8

Molecular Formula: C₂₁H₂₄O₁₁

Molecular Weight: 452.414

Accurate Mass: 452.131865

Percentage Composition: C 55.75%; H 5.35%; O 38.90%

Biological Source: Isol. from *Davallia divaricata*

Optical Rotation: [α]_D –30 (MeOH)