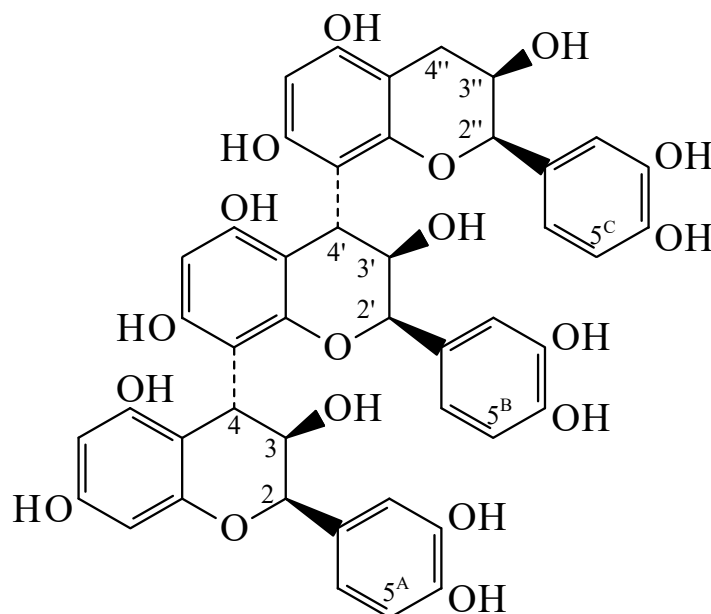




>>Entry Name: [3,3',4',5,7-Pentahydroxyflavan(4→8)]₂-3,3',4',5,7-pentahydroxyflavan

ENTRY UNDER REVIEW

Synonym(s): 2,2',2''-Tris(3,4-dihydroxyphenyl)-3,3',3'',4,4',4''-hexahydro-[4,8':4',8''-ter-2*H*-1-benzopyran]-3,3',3'',5,5',5'',7,7',7''-nonol, 9Cl



(2*R*,2'*R*,2''*R*,3*R*,3'*R*,3''*R*,4*R*,4'*R*)-form

CAS Registry Number: 37064-30-5

Related CAS Registry Numbers(s): 23459-99-6 78655-09-1 80823-25-2

Molecular Formula: C₄₅H₃₈O₁₈

Molecular Weight: 866.784

Accurate Mass: 866.20582

Percentage Composition: C 62.36%; H 4.42%; O 33.23%

>>Variant: (2*R*,2'*R*,2''*R*,3*R*,3'*R*,3''*R*,4*R*,4'*R*)-form

Synonym(s): [Epicatechin(4β→8)]₂epicatechin. Proanthocyanidin C₁. Procyanidin C₁

CAS Registry Number: 65085-09-8

Molecular Formula: C₄₅H₃₈O₁₈

Molecular Weight: 866.784

Accurate Mass: 866.20582

Percentage Composition: C 62.36%; H 4.42%; O 33.23%

Biological Source: Widespread in plant spp.

Optical Rotation: [α]_D +102 (H₂O)

>>Derivative: 3',3''-Bis(3,4,5-trihydroxybenzoyl)

Synonym(s): Procyanidin C1 3',3''-di-*O*-gallate

CAS Registry Number: 106533-61-3

Molecular Formula: C₅₉H₄₆O₂₆

Molecular Weight: 1170.997

Accurate Mass: 1170.22774

Percentage Composition: C 60.52%; H 3.96%; O 35.52%

Biological Source: Isol. from *Rheum* sp. (commercial rhubarb)

Physical Description: Tan amorph. powder + 4H₂O

Optical Rotation: [α]_D²⁸ -5.5 (c, 0.64 in Me₂CO)

>>Derivative: 3,3',3''-Tris(3,4,5-trihydroxybenzoyl)

Synonym(s): Procyanidin C1 3,3',3''-tri-*O*-gallate

CAS Registry Number: 106533-62-4

Molecular Formula: C₆₆H₅₀O₃₀

Molecular Weight: 1323.103

Accurate Mass: 1322.2387

Percentage Composition: C 59.91%; H 3.81%; O 36.28%

Biological Source: Isol. from *Rheum* sp.

Physical Description: Tan amorph. powder + 3H₂O

Optical Rotation: [α]