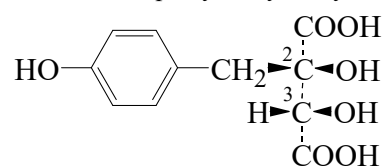




>>Entry Name: Piscidic acid

Synonym(s): 2,3-Dihydroxy-2-[(4-hydroxyphenyl)methyl]butanedioic acid, 9Cl. *p*-Hydroxybenzyltartaric acid



Molecular Formula: C₁₁H₁₂O₇

Molecular Weight: 256.212

Accurate Mass: 256.058305

Percentage Composition: C 51.57%; H 4.72%; O 43.71%

Other Data: All 4 stereoisomers have been synthesised

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

CAS Registry Number: 35388-57-9

Molecular Formula: C₁₁H₁₂O₇

Molecular Weight: 256.212

Accurate Mass: 256.058305

Percentage Composition: C 51.57%; H 4.72%; O 43.71%

Biological Source: Isol. from bark of *Piscidia erythrina*, from *Narcissus poeticus*, *Cimicifuga simplex*, *Agave americana* and *Opuntia ficus-indica*

Physical Description: Elongated prisms (EtOAc/CHCl₃)

Melting Point: Mp 186-187°

Optical Rotation: [α]_D +42.8 (c, 0.8 in MeOH)

UV: [neutral] λ_{max} 255 (log ε 3.88); 277 (log ε 3.17) (MeOH)

>>Derivative: Di-Me ester

Molecular Formula: C₁₃H₁₆O₇

Molecular Weight: 284.265

Accurate Mass: 284.089605

Percentage Composition: C 54.93%; H 5.67%; O 39.40%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 127°

Optical Rotation: [α]_D¹⁹ +23.71 (c, 6.37 in EtOH)

>>Derivative: 3-*O*-(3,4-Dihydroxy-*E*-cinnamoyl)

Synonym(s): 3-*O*-Caffeoylpiscidic acid. 2-*O*-Caffeoylpiscidic acid. **Cimicifugic acid D**

CAS Registry Number: 219986-51-3

Molecular Formula: C₂₀H₁₈O₁₀

Molecular Weight: 418.356

Accurate Mass: 418.09

Percentage Composition: C 57.42%; H 4.34%; O 38.24%

Biological Source: Constit. of *Cimicifuga simplex*

Physical Description: Pale yellow powder

Optical Rotation: [α]_D +67.3 (c, 0.34 in MeOH)

UV: [neutral] λ_{max} 248 (sh) (log ε 4.02); 291 (log ε 4.07); 332 (log ε 4.25) (MeOH)

>>Derivative: 3-*O*-(3-Hydroxy-4-methoxy-*E*-cinnamoyl)

Synonym(s): 3-*O*-Isoferuloylpiscidic acid. 2-*O*-Isoferuloylpiscidic acid. **Cimicifugic acid F**

CAS Registry Number: 220618-91-7

Molecular Formula: C₂₁H₂₀O₁₀

Molecular Weight: 432.383

Accurate Mass: 432.10565

Percentage Composition: C 58.34%; H 4.66%; O 37.00%

Biological Source: Constit. of *Cimicifuga simplex*

Physical Description: Pale yellow powder

Optical Rotation: [α]_D +37.6 (c, 0.5 in MeOH)

UV: [neutral] λ_{max} 245 (sh) (log ε 4.1); 297 (log ε 4.19); 326 (log ε 4.25) (MeOH)