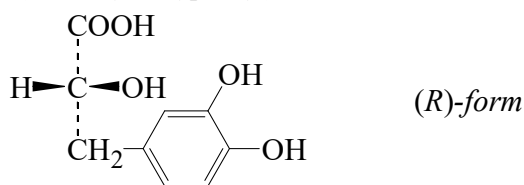




>>Entry Name: 3-(3,4-Dihydroxyphenyl)-2-hydroxypropanoic acid

Synonym(s): α ,3,4-Trihydroxybenzenepropanoic acid, 9CI. 3-(3,4-Dihydroxyphenyl)lactic acid. Dan Shen Su



CAS Registry Number: 23028-17-3

Related CAS Registry Numbers(s): 42085-50-7 67810-33-7 67920-52-9 69339-96-4 81075-52-7

Molecular Formula: $C_9H_{10}O_5$

Molecular Weight: 198.175

Accurate Mass: 198.052825

Percentage Composition: C 54.55%; H 5.09%; O 40.37%

>>Variant: (R)-form

CAS Registry Number: 76822-21-4

Type of Compound Code(s): VG0060

Molecular Formula: $C_9H_{10}O_5$

Molecular Weight: 198.175

Accurate Mass: 198.052825

Percentage Composition: C 54.55%; H 5.09%; O 40.37%

Biological Source: Constit. of *Coptidis rhizoma* and *Salvia miltiorrhiza*

Use/Importance: Coronary vasodilator

Physical Description: Prisms (EtOAc/ C_6H_6)

Melting Point: Mp 84-87°

Optical Rotation: $[\alpha]_D^{18} +10.8$ (c, 3.7 in MeOH)

>>Derivative: 4'-O- β -D-Glucopyranoside

CAS Registry Number: 96552-85-1

Type of Compound Code(s): VG0060

Molecular Formula: $C_{15}H_{20}O_{10}$

Molecular Weight: 360.317

Accurate Mass: 360.10565

Percentage Composition: C 50.00%; H 5.59%; O 44.40%

Biological Source: Constit. of *Coptidis rhizoma*

Physical Description: Hygroscopic powder

Optical Rotation: $[\alpha]_D^{25} -41$ (c, 1.00 in MeOH)

>>Derivative: 2-O-(4-Hydroxy-*E*-cinnamoyl)

Synonym(s): Isorinic acid

Molecular Formula: $C_{18}H_{16}O_7$

Molecular Weight: 344.32

Accurate Mass: 344.089605

Percentage Composition: C 62.79%; H 4.68%; O 32.53%

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D +82.5$ (c, 1 in MeOH)

Other Data: Isol. as glucoside

>>Derivative: 2-O-(4-Hydroxy-*E*-cinnamoyl), 4'-O- β -D-glucopyranoside

Type of Compound Code(s): VG0060

Molecular Formula: $C_{24}H_{26}O_{12}$

Molecular Weight: 506.462

Accurate Mass: 506.14243

Percentage Composition: C 56.92%; H 5.17%; O 37.91%

Biological Source: Constit. of the fruit of *Helicteres isora*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D -16$ (c, 0.3 in H_2O)

UV: [neutral] λ_{max} 219 (log ϵ 4.26); 286 (log ϵ 4.16); 319 (log ϵ 4.07) (MeOH)