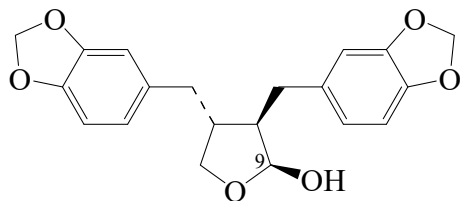




>>Entry Name: Cubebin

Synonym(s): 3,4-Bis(1,3-benzodioxol-5-ylmethyl)tetrahydro-2-furanol, 9Cl. 9-Hydroxy-3,4:3',4'-bis(methylenedioxy)-9,9'-epoxylignan. β -Cubebin



CAS Registry Number: 18423-69-3

Related CAS Registry Numbers(s): 112448-61-0 112448-62-1

Molecular Formula: $C_{20}H_{20}O_6$

Molecular Weight: 356.374

Accurate Mass: 356.12599

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Biological Source: Isol. from unripe fruit of *Piper cubeba*, also from *Aristolochia* spp., *Virola* spp. and other plants

Use/Importance: Shows urinary stimulant props.

Physical Description: Cryst. (EtOH or C_6H_6)

Melting Point: Mp 131-132°

Optical Rotation: $[\alpha]_D^{14} -17.1$ (Me_2CO). $[\alpha]_D^{14} -45.7$ ($CHCl_3$)

Other Data: Readily epimerises at C-9

>>Derivative: Et ether

Synonym(s): *O*-Ethylcubebin

CAS Registry Number: 146830-09-3

Molecular Formula: $C_{22}H_{24}O_6$

Molecular Weight: 384.428

Accurate Mass: 384.15729

Percentage Composition: C 68.74%; H 6.29%; O 24.97%

Biological Source: Constit. of *Piper cubeba* and *Piper clusii*

Physical Description: Visc. solid

>>Derivative: 9-Epimer

Synonym(s): α -Cubebin

CAS Registry Number: 112458-74-9

Molecular Formula: $C_{20}H_{20}O_6$

Molecular Weight: 356.374

Accurate Mass: 356.12599

Percentage Composition: C 67.41%; H 5.66%; O 26.94%

Biological Source: Constit. of *Aristolochia birostris*

>>Derivative: Me ether

Synonym(s): 9-Methoxy-3,4:3',4'-bis(methylenedioxy)-9,9'-epoxylignan. *O*-Methyl- β -cubebin

Molecular Formula: $C_{21}H_{22}O_6$

Molecular Weight: 370.401

Accurate Mass: 370.14164

Percentage Composition: C 68.10%; H 5.99%; O 25.92%

Biological Source: Constit. of *Virola surinamensis*

Physical Description: Amorph. solid

Optical Rotation: $[\alpha]_D -2.2$ (c, 0.2 in $CHCl_3$)

>>Derivative: 9-Epimer, Me ether

Synonym(s): *O*-Methyl- α -cubebin

Molecular Formula: $C_{21}H_{22}O_6$

Molecular Weight: 370.401

Accurate Mass: 370.14164

Percentage Composition: C 68.10%; H 5.99%; O 25.92%

Biological Source: Constit. of *Virola surinamensis*

Physical Description: Oil

Optical Rotation: $[\alpha]_D -17.9$ (c, 0.2 in $CHCl_3$)