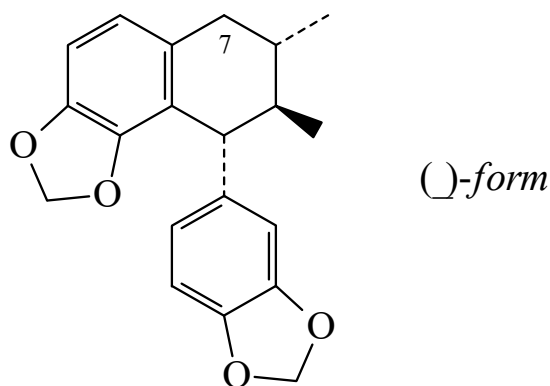




>>Entry Name: Otobain

ENTRY UNDER REVIEW

Synonym(s): 3,4:3',4'-Bis(methylenedioxy)-2,7'-cyclo lignan. Otobite



Molecular Formula: C₂₀H₂₀O₄

Molecular Weight: 324.376

Accurate Mass: 324.13616

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

>>Variant: (–)-form

CAS Registry Number: 3738-01-0

Molecular Formula: C₂₀H₂₀O₄

Molecular Weight: 324.376

Accurate Mass: 324.13616

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

Biological Source: Isol. from fruits of *Myristica otoba* and *Myristica simarum*

Physical Description: Cryst. (petrol)

Melting Point: Mp 136-137°

Optical Rotation: [α]_D –43 (c, 0.8 in CHCl₃)

>>Derivative: 7-Oxo

Synonym(s): Otobanone. 7-Oxootobain

CAS Registry Number: 34426-79-4

Molecular Formula: C₂₀H₁₈O₅

Molecular Weight: 338.359

Accurate Mass: 338.115425

Percentage Composition: C 71.00%; H 5.36%; O 23.64%

Biological Source: Isol. from *Myristica simarum* and from nutmeg (*Myristica fragrans*)

Melting Point: Mp 175-176°

Optical Rotation: [α]_D –27.1 (c, 0.7 in CHCl₃)

>>Variant: (+)-form

Molecular Formula: C₂₀H₂₀O₄

Molecular Weight: 324.376

Accurate Mass: 324.13616

Percentage Composition: C 74.06%; H 6.21%; O 19.73%

>>Derivative: 5-Methoxy, 7',8'*R*-didehydro

Synonym(s): 5-Methoxy-3,4:3',4'-bis(methylenedioxy)-2,7'-cyclo lign-7'-ene

CAS Registry Number: 98767-35-2

Molecular Formula: C₂₁H₂₀O₅

Molecular Weight: 352.386

Accurate Mass: 352.131075

Percentage Composition: C 71.58%; H 5.72%; O 22.70%

Biological Source: Constit. of *Virola calophylloidea*

Physical Description: Cryst. (MeOH)

Melting Point: Mp 152°

Optical Rotation: [α]_D²⁰ +51.7 (c, 0.8 in CHCl₃)

UV: [neutral] $\lambda_{\max}$ 279 (ϵ 1200); 292 (ϵ 1050); 332 (ϵ 300) (MeOH)