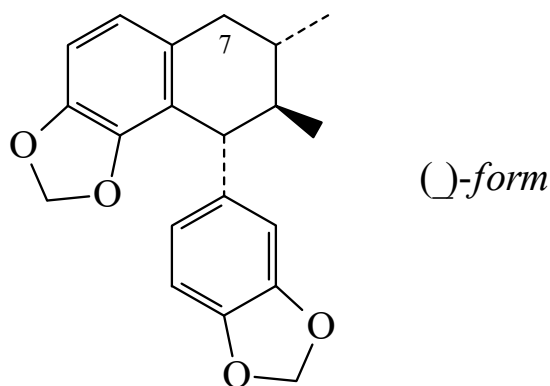




>>Entry Name: Otobain

ENTRY UNDER REVIEW

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



**Molecular Formula:** C<sub>20</sub>H<sub>20</sub>O<sub>4</sub>

**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:** C<sub>20</sub>H<sub>20</sub>O<sub>4</sub>

**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:** [ $\alpha$ ]<sub>D</sub> –43 (c, 0.8 in CHCl<sub>3</sub>)

>>Derivative: 7-Oxo

Synonym(s): Otobanone. 7-Oxootobain

**CAS Registry Number:** 34426-79-4

**Molecular Formula:** C<sub>20</sub>H<sub>18</sub>O<sub>5</sub>

**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:** [ $\alpha$ ]<sub>D</sub> –27.1 (c, 0.7 in CHCl<sub>3</sub>)

>>Variant: (+)-form

**Molecular Formula:** C<sub>20</sub>H<sub>20</sub>O<sub>4</sub>

**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:** C<sub>21</sub>H<sub>20</sub>O<sub>5</sub>

**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:** [ $\alpha$ ]<sub>D</sub><sup>20</sup> +51.7 (c, 0.8 in CHCl<sub>3</sub>)

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