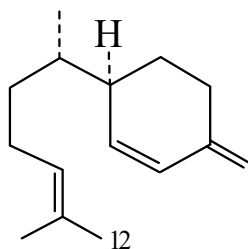




>>Entry Name: 1,3(15),10-Bisabolatriene

ENTRY UNDER REVIEW

Synonym(s): 3-(1,5-Dimethyl-4-hexenyl)-6-methylenecyclohexene, 9Cl. β -Sesquiphellandrene



CAS Registry Number: 20307-83-9

Molecular Formula: $C_{15}H_{24}$

Molecular Weight: 204.355

Accurate Mass: 204.1878

Percentage Composition: C 88.16%; H 11.84%

Biological Source: Constit. of the oil of ginger (*Zingiber officinale*)

Physical Description: Oil

Boiling Point: Bp_1 90°

Optical Rotation: $[\alpha]_D^{20}$ -3.99 (neat)

>>Derivative: Nitrosite

Molecular Formula: $C_{15}H_{24}N_2O_3$

Molecular Weight: 280.366

Percentage Composition: C 64.26%; H 8.63%; N 9.99%; O 17.12%

Physical Description: Cryst. (Me_2CO)

Melting Point: Mp 88-90 dec.°

Optical Rotation: $[\alpha]_D^{20}$ +29 (c, 1.5 in $CHCl_3$)

>>Derivative: 10 ξ ,11 ξ -Epoxide

Synonym(s): 10,11-Epoxy-1,3(15)-bisaboladiene. 10,11-Epoxy- β -sesquiphellandrene

CAS Registry Number: 80442-54-2

Molecular Formula: $C_{15}H_{24}O$

Molecular Weight: 220.354

Accurate Mass: 220.182715

Percentage Composition: C 81.76%; H 10.98%; O 7.26%

Biological Source: Constit. of *Stylotrichum rotundifolium*

Physical Description: Oil

>>Derivative: 12-Oxo

Synonym(s): 1,3(15),10-Bisabolatrien-12-al. 12-Oxo- β -sesquiphellandrene

CAS Registry Number: 71939-69-0

Molecular Formula: $C_{15}H_{22}O$

Molecular Weight: 218.338

Accurate Mass: 218.167065

Percentage Composition: C 82.52%; H 10.16%; O 7.33%

Biological Source: Constit. of *Tarchonanthus trilobus*

Physical Description: Oil

Optical Rotation: $[\alpha]_D$ -9.3 (c, 0.15 in $CHCl_3$)

References:

- Connell, D.W. *et al.*, *Aust. J. Chem.*, 1966, **19**, 283, (β -Sesquiphellandrene)
Bohlmann, F. *et al.*, *Phytochemistry*, 1979, **18**, 677, (12-Oxo- β -sesquiphellandrene)
Bohlmann, F. *et al.*, *Phytochemistry*, 1981, **20**, 1887, (Epoxybisaboladiene)
Kreiser, W. *et al.*, *Helv. Chim. Acta*, 1999, **82**, 1427-1433, (*synth*)