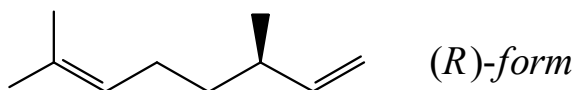




>>Entry Name: 3,7-Dimethyl-1,6-octadiene

Synonym(s): β -Linalolene. Citronellene



CAS Registry Number: 2436-90-0

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Hazard & Toxicity: Skin irritant

Fluka: 27475

>>Variant: (R)-form

Type of Compound Code(s): VS0100

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Biological Source: Degradn. prod. of Zingiberene

Physical Description: Oil

Boiling Point: Bp 158-159°

Optical Rotation: $[\alpha]_D^{22} +8.7$

>>Variant: ($\pm$)-form

Molecular Formula: C₁₀H₁₈

Molecular Weight: 138.252

Accurate Mass: 138.14085

Percentage Composition: C 86.88%; H 13.12%

Boiling Point: Bp₇₂₀ 155-156°

Density: $d_4^{18} 0.761$

Refractive Index: $n_D^{18} 1.4385$

References:

Daniewski, W. *et al.*, *Pol. J. Chem. (Rocz. Chem.)*, 1971, **45**, 923, (*synth*)

Rienaecker, R., *Chimia*, 1973, **27**, 97, (*synth*)

Watanabe, S. *et al.*, *J. Appl. Chem. Biotechnol.*, 1974, **24**, 639, (*synth*)

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