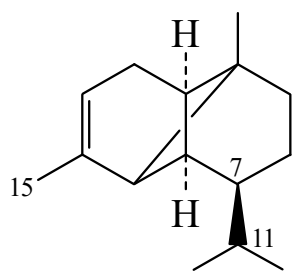




>>Entry Name: 3-Copaene

Synonym(s): 1,3-Dimethyl-8-(1-methylethyl)tricyclo[4.4.0.0^{2,7}]dec-3-ene, 9Cl. 8-Isopropyl-1,3-dimethyltricyclo[4.4.0.0^{2,7}]dec-3-ene



(1aH,6aH,7aH)-form

Related CAS Registry Numbers(s): 41530-63-6 41530-64-7 115728-41-1

Molecular Formula: C₁₅H₂₄

Molecular Weight: 204.355

Accurate Mass: 204.1878

Percentage Composition: C 88.16%; H 11.84%

>>Variant: (1αH,6αH,7αH)-form

Synonym(s): Ylangene. α-Ylangene

CAS Registry Number: 14912-44-8

Molecular Formula: C₁₅H₂₄

Molecular Weight: 204.355

Accurate Mass: 204.1878

Percentage Composition: C 88.16%; H 11.84%

Biological Source: Isol. from various essential oils, esp. *Schizandra chinensis*

Physical Description: Oil

Optical Rotation: [α]_D²⁰+50.5

>>Variant: (1βH,6βH,7αH)-form

Synonym(s): α-Copaene. Aglaiene. Copaene

CAS Registry Number: 3856-25-5

Molecular Formula: C₁₅H₂₄

Molecular Weight: 204.355

Accurate Mass: 204.1878

Percentage Composition: C 88.16%; H 11.84%

Biological Source: Constit. of the oils of African Copaiva balsam and *Sindora wallichii*. Also from various other higher plant oils and from the brown alga *Dictyopteris divaricata*

Physical Description: Oil

Boiling Point: Bp 246-251°

Optical Rotation: [α]_D −13.3 (CHCl₃)

Other Data: *n*_D²⁰ 1.4722

Fluka: 27814

>>Derivative: 11-Hydroxy

Synonym(s): 3-Copaen-11-ol. α-Copaen-11-ol

CAS Registry Number: 41370-56-3

Molecular Formula: C₁₅H₂₄O

Molecular Weight: 220.354

Accurate Mass: 220.182715

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

Biological Source: Constit. of the essential oil of *Parabenzoin praecox*

Physical Description: Cryst.

Melting Point: Mp 99.5-100.5°

Optical Rotation: [α]_D +9.2 (CHCl₃)