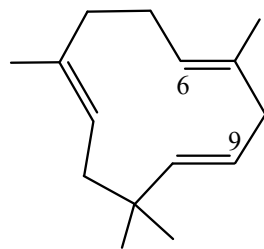




>>Entry Name: 2,6,9-Humulatriene

ENTRY UNDER REVIEW

Synonym(s): 2,6,6,9-Tetramethyl-1,4,8-cycloundecatriene. α -Humulene. α -Caryophyllene (obsol.). Humulene



CAS Registry Number: 6753-98-6

Molecular Formula: C₁₅H₂₄

Molecular Weight: 204.355

Accurate Mass: 204.1878

Percentage Composition: C 88.16%; H 11.84%

Biological Source: Constit. of many essential oils including hops (*Humulus lupulus*) and cloves (*Syzygium aromaticum*)

Physical Description: Oil

Boiling Point: Bp₁₀ 123°

Fluka: 53675

Sigma: H5887

>>Derivative: AgNO₃ complex

Physical Description: Cryst. (EtOH)

Melting Point: Mp 175°

>>Derivative: 6,7-Episulfide

Synonym(s): 1,5,5,8-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene, 9Cl

CAS Registry Number: 65563-96-4

Molecular Formula: C₁₅H₂₄S

Molecular Weight: 236.421

Accurate Mass: 236.15987

Percentage Composition: C 76.21%; H 10.23%; S 13.56%

Biological Source: Constit. of hops

Physical Description: Oil

>>Derivative: 9,10-Episulfide

Synonym(s): 3,7,7,10-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene, 9Cl

CAS Registry Number: 74841-84-2

Molecular Formula: C₁₅H₂₄S

Molecular Weight: 236.421

Accurate Mass: 236.15987

Percentage Composition: C 76.21%; H 10.23%; S 13.56%

Biological Source: Constit. of hops

Physical Description: Oil

References:

McPhail, A.T. *et al.*, *J.C.S.(B)*, 1966, 112, (*cryst struct*)

Dev, S. *et al.*, *J.A.C.S.*, 1968, **90**, 1246, (*pmr*)

Karrer, W. *et al.*, *Konstitution und Vorkommen der Organischen Pflanzenstoffe*, 2nd edn., Birkhäuser Verlag, Basel, 1972, no. 1929, (*occur*)

Cradwick, M.E. *et al.*, *J.C.S. Perkin 2*, 1973, 404, (*conformn*)

Vig, O.P. *et al.*, *Indian J. Chem., Sect. B*, 1976, **14**, 855, (*synth*)

Kitagawa, Y. *et al.*, *J.A.C.S.*, 1977, **99**, 3864, (*synth*)

Peppard, T.L. *et al.*, *J.C.S. Perkin 1*, 1980, 311, (*isol*)

McMurry, J.E. *et al.*, *Tet. Lett.*, 1982, **23**, 2723, (*synth*)

Shirahama, H. *et al.*, *Chem. Lett.*, 1983, 281, (*synth*)

McMurry, J.E. *et al.*, *Tetrahedron*, 1987, **43**, 5489, (*synth*)

Corey, E.J. *et al.*, *Tet. Lett.*, 1993, **34**, 3675, (*synth*)