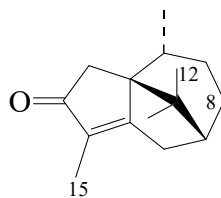




>>Entry Name: 4-Patchoulen-3-one

Synonym(s): Cyperotundone. Cyperenone. Articulone. Isopatchoulenone



CAS Registry Number: 3466-15-7

Molecular Formula: C₁₅H₂₂O

Molecular Weight: 218.338

Accurate Mass: 218.167065

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

Biological Source: Constit. of *Cyperus scariosus*, *Cyperus rotundus* and *Cyperus articulatus*

Physical Description: Cryst. (petrol)

Melting Point: Mp 46-47.5°

Boiling Point: Bp_{0.5} 136-138°

Optical Rotation: [α]_D +40.4 (c, 3.2 in CHCl₃)

UV: [neutral] λ_{max} 244 () (EtOH) (Berdy)

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Red cryst. (EtOH)

Melting Point: Mp 231-232°

>>Derivative: 8α-Hydroxy

Synonym(s): 8-Hydroxy-4-patchoulen-3-one. **8-Hydroxycyperotundone**

Molecular Formula: C₁₅H₂₂O₂

Molecular Weight: 234.338

Accurate Mass: 234.16198

Percentage Composition: C 76.88%; H 9.46%; O 13.66%

Biological Source: Isol. from *Jungia polita*

Physical Description: Gum

>>Derivative: 12,15-Diacetoxy

Synonym(s): 12,15-Diacetoxycyperenone

CAS Registry Number: 98211-44-0

Molecular Formula: C₁₉H₂₆O₅

Molecular Weight: 334.411

Accurate Mass: 334.178025

Percentage Composition: C 68.24%; H 7.84%; O 23.92%

Biological Source: Constit. of *Moschardia pinnatifida*

Physical Description: Oil

>>Derivative: 15-(3-Hydroxy-3-methylbutanoyloxy)

CAS Registry Number: 98211-43-9

Molecular Formula: C₂₀H₃₀O₄

Molecular Weight: 334.455

Accurate Mass: 334.21441

Percentage Composition: C 71.82%; H 9.04%; O 19.13%

Biological Source: Constit. of *Moschardia pinnatifida*

Physical Description: Oil

References:

Hikino, H. *et al.*, *Tetrahedron*, 1967, **23**, 2169, (*struct*)

Hikino, H. *et al.*, *Chem. Pharm. Bull.*, 1968, **66**, 43, (*synth*)

Neville, G.A. *et al.*, *Tetrahedron*, 1968, **24**, 3891, (*pmr, ms, bibl*)

Singh, P. *et al.*, *Phytochemistry*, 1985, **24**, 1525-1529, (*deriv*)

Ybarra, M.I. *et al.*, *Phytochemistry*, 1992, **31**, 3627, (*8-Hydroxycyperotundone*)