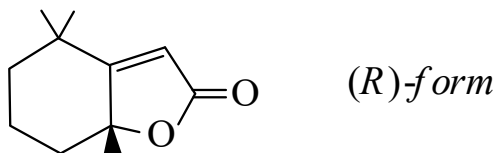




>>Entry Name: 5,6,7,7a-Tetrahydro-4,4,7a-trimethyl-2(4H)-benzofuranone, 9CI

ENTRY UNDER REVIEW

Synonym(s): 2-Hydroxy-2,6,6-trimethylcyclohexylidene-1-acetic acid lactone. Dihydroactinidiolide



CAS Registry Number: 15356-74-8

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Biological Source: Has been isolated from tobacco, tea, coffee, fruits and animal glands

Use/Importance: An important aroma constit. of cigar tobacco and tea

Other Data: The prod. from plant sources is largely racemic (from tobacco (R)-isomer of 30% ee, from *A. polygama* (S)-isomer of 6% ee)

>>Variant: (R)-form

CAS Registry Number: 38273-56-2

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Use/Importance: Bioactive as a component of the queen recognition pheromone of *Solenopsis invicta* (red imported fire ant)

Melting Point: Mp 41°. Mp 69-71°

Optical Rotation: $[\alpha]_D^{20} -119.9$ (c, 0.01 in CHCl₃)

>>Variant: (S)-form

CAS Registry Number: 17092-92-1

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Biological Source: Constit. of the leaves of *Actinidia polygama*

Use/Importance: Shows physiological activity towards the cat family

Melting Point: Mp 71-72° (40-41°)

Optical Rotation: $[\alpha]_D^{15} +7.1$ (natural). $[\alpha]_D^{22} +122.7$ (CHCl₃) (synthetic)

Other Data: Not active as a fire ant pheromone

>>Variant: (±)-form

CAS Registry Number: 19432-05-4

Molecular Formula: C₁₁H₁₆O₂

Molecular Weight: 180.246

Accurate Mass: 180.11503

Percentage Composition: C 73.30%; H 8.95%; O 17.75%

Physical Description: Cryst. (Et₂O/petrol at -15°)

Melting Point: Mp 42°

Boiling Point: Bp_{0.001} 90°

References:

- Mousseron-Canet, M. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 608, (*synth*)
Sakan, T. *et al.*, *Tet. Lett.*, 1967, 1623, (*isol, synth*)
Isoe, S. *et al.*, *Tet. Lett.*, 1972, 2517, (*abs config*)
Eschenmoser, W. *et al.*, *Helv. Chim. Acta*, 1975, **58**, 1722, (*synth*)
Kienzle, F. *et al.*, *Helv. Chim. Acta*, 1978, **61**, 2616, (*synth*)
Chakraborty, T.K. *et al.*, *Tet. Lett.*, 1984, **25**, 2895, (*synth*)
Mori, K. *et al.*, *Tetrahedron*, 1986, **42**, 283, (*synth*)
Cain, C.M. *et al.*, *Tet. Lett.*, 1987, **28**, 3723, (*synth*)
Subbaraju, G.V. *et al.*, *Tet. Lett.*, 1991, **32**, 4871, (*synth*)
Mori, K. *et al.*, *Annalen*, 1993, 77, (*synth*)
Irie, O. *et al.*, *Chem. Lett.*, 1995, 53, (*synth*)