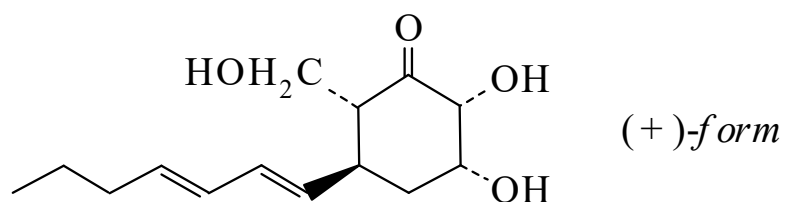




>>Entry Name: Palitantin

Synonym(s): 3-(1,3-Heptadienyl)-5,6-dihydroxy-2-(hydroxymethyl)cyclohexanone, 9Cl



Molecular Formula: C₁₄H₂₂O₄

Molecular Weight: 254.325

Accurate Mass: 254.15181

Percentage Composition: C 66.12%; H 8.72%; O 25.16%

>>Variant: (+)-form

CAS Registry Number: 15265-28-8

Molecular Formula: C₁₄H₂₂O₄

Molecular Weight: 254.325

Accurate Mass: 254.15181

Percentage Composition: C 66.12%; H 8.72%; O 25.16%

Biological Source: Metab. of various *Penicillium* spp.

Use/Importance: Has antifungal activity

Melting Point: Mp 164-165° (157-158°)

Optical Rotation: [α]_D +2 (c, 1.1 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; fairly sol. H₂O, Et₂O; poorly sol. hexane

UV: [neutral] λ_{max} 232 () (MeOH) (Berdy) [neutral] λ_{max} 232 (ε 34000) (EtOH) (Berdy) [neutral] λ_{max} 234 (ε 28840); 269 (ε 830); 280 (ε 616) (dioxan) (Berdy)

>>Variant: (±)-form

CAS Registry Number: 66211-90-3

Molecular Formula: C₁₄H₂₂O₄

Molecular Weight: 254.325

Accurate Mass: 254.15181

Percentage Composition: C 66.12%; H 8.72%; O 25.16%

Physical Description: Cryst. (H₂O)

Melting Point: Mp 139-141°

References:

- Haerri, E. *et al.*, *Helv. Chim. Acta*, 1963, **46**, 1235, (*isol*)
Grove, J.F. *et al.*, *J.C.S.*, 1964, 3497, (*abs config, pmr*)
Austin, A.T. *et al.*, *Chem. Ind. (London)*, 1966, 1228, (*uv*)
Ichihara, A. *et al.*, *Tetrahedron*, 1980, **36**, 1547, (*synth*)
Demetriadou, A.K. *et al.*, *J.C.S. Perkin 1*, 1988, 773, (*biosynth, pmr, cmr, O-18 nmr, bibl*)
Hanessian, S. *et al.*, *Tetrahedron*, 1989, **45**, 6623, (*synth*)
Deruyttere, X. *et al.*, *Synlett*, 1992, 51, (*synth*)
Hareau, G. *et al.*, *Tet. Lett.*, 1999, **40**, 7493-7496, (*synth, pmr, cmr*)