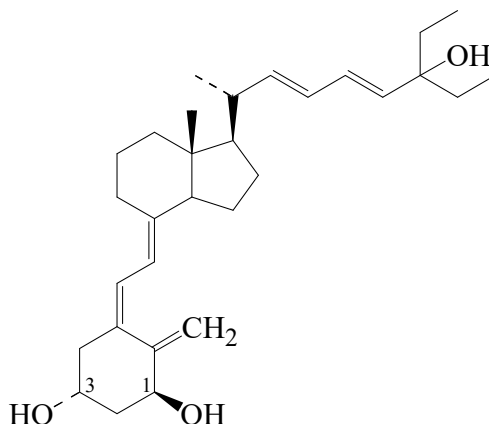




>>Entry Name: Secocalcitol, INN

Synonym(s): 5-[[1-(6-Ethyl-6-hydroxy-1-methyl-2,4-octadienyl)octahydro-7a-methyl-4H-inden-4-ylidene]ethylidene]-4-methylene-1,3-cyclohexanediol, 9CI. 24a,26a,27a-Trihomo-9,10-secocholesta-5,7,10(19),22,24-pentaene-1,3,25-triol



CAS Registry Number: 134404-52-7

Related CAS Registry Numbers(s): 134523-49-2

Molecular Formula: C₃₀H₄₆O₃

Molecular Weight: 454.692

Accurate Mass: 454.344695

Percentage Composition: C 79.25%; H 10.20%; O 10.56%

Biological Use/Importance: Vitamin D analogue. Antineoplastic agent, antiproliferative agent. Induces apoptosis in a human breast cancer cell line

Physical Description: Needles (methyl formate/hexane)

Development Status: Phase I clin. trials for treatment of breast and colon cancer completed (1997)

UV: [neutral] λ_{max} 232 (ε 43745); 264 (ε 18060) (EtOH)

Other Data: Stereochem. is (1R,3S,5Z,7E,22E,24E)

References:

- Pat. Coop. Treaty (WIPO)*, 1991, *Leo*, 91 00 855; *CA*, **115**, 50097a, (*synth, pharmacol*)
Maenpaa, P.H. *et al.*, *Ann. N.Y. Acad. Sci.*, 1995, **761**, 349-350, (*pharmacol*)
Mahonen, A. *et al.*, *Biochem. Pharmacol.*, 1996, **51**, 887-892, (*pharmacol*)
Puthier, D. *et al.*, *Blood*, 1996, **88**, 4659-4666, (*pharmacol*)
Shankar, V.N. *et al.*, *Biochem. Pharmacol.*, 1997, **53**, 783-793, (*metab*)
Hansen, C.M. *et al.*, *Biochem. Pharmacol.*, 1997, **54**, 1173-1179, (*pharmacol, rev*)
Falzon, M. *et al.*, *Endocrinology (Baltimore)*, 1998, **139**, 1046-1053, (*pharmacol*)
VanWeelden, K. *et al.*, *Endocrinology (Baltimore)*, 1998, **139**, 2102-2110, (*pharmacol*)
Wu, G. *et al.*, *J. Biol. Chem.*, 1998, **273**, 7749-7756, (*pharmacol*)