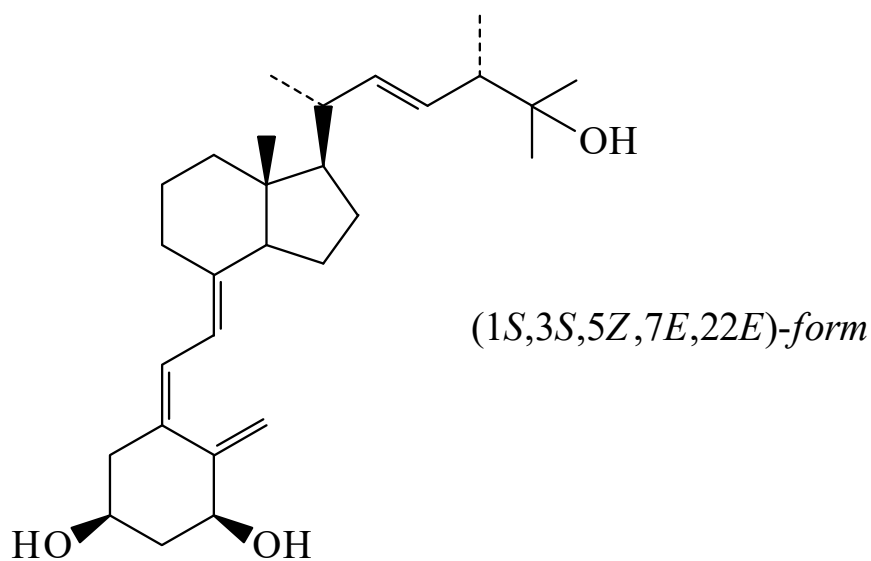




>>Entry Name: 9,10-Secoergosta-5,7,10(19),22-tetraene-1,3,25-triol, 9CI



Related CAS Registry Numbers(s): 55248-15-2 73837-25-9 95783-09-8 98117-32-9 98169-40-5 98169-41-6 98169-42-7 111422-23-2 111467-50-6

Molecular Formula: C₂₈H₄₄O₃

Molecular Weight: 428.654

Accurate Mass: 428.329045

Percentage Composition: C 78.46%; H 10.35%; O 11.20%

Other Data: Deuterated, fluorinated and tritiated compds. have been synth.

>>Variant: (1S,3R,5Z,7E,22E)-form

Synonym(s): 1 α ,25-Dihydroxyvitamin D₂. Ercalcitriol

CAS Registry Number: 60133-18-8

Molecular Formula: C₂₈H₄₄O₃

Molecular Weight: 428.654

Accurate Mass: 428.329045

Percentage Composition: C 78.46%; H 10.35%; O 11.20%

Use/Importance: Metab. and suggested active form of vitamin D₂. Stimulates Ca transport in gastrointestinal tract

Physical Description: Cryst. (methyl formate)

Melting Point: Mp 169-170°

Optical Rotation: [α]_D²⁵ +47.2 (c,0.2 in EtOH)

>>Variant: (1S,3R,5Z,7E,22E,24R)-form

CAS Registry Number: 95783-08-7

Molecular Formula: C₂₈H₄₄O₃

Molecular Weight: 428.654

Accurate Mass: 428.329045

Percentage Composition: C 78.46%; H 10.35%; O 11.20%

Physical Description: Oil

References:

- Sicinski, R.R. *et al.*, *Bioorg. Chem.*, 1985, **13**, 158, (*synth, isomers*)
Baggiolini, E.G. *et al.*, *J.O.C.*, 1986, **51**, 3098, (*synth*)
Synform, 1986, **4**, 250, (*rev, synth*)
Sicinski, R.R. *et al.*, *Anal. Biochem.*, 1987, **161**, 96, (*synth, labelled cpds*)
DeLuca, H.F. *et al.*, *Am. J. Physiol.*, 1988, **254**, E402, (*props*)
Kutner, A. *et al.*, *J.O.C.*, 1988, **53**, 3450, (*synth*)
Kiegel, J. *et al.*, *Tet. Lett.*, 1991, **32**, 6057, (*synth*)
Torreiro, M. *et al.*, *J.O.C.*, 1997, **62**, 6344-6352, (*synth*)