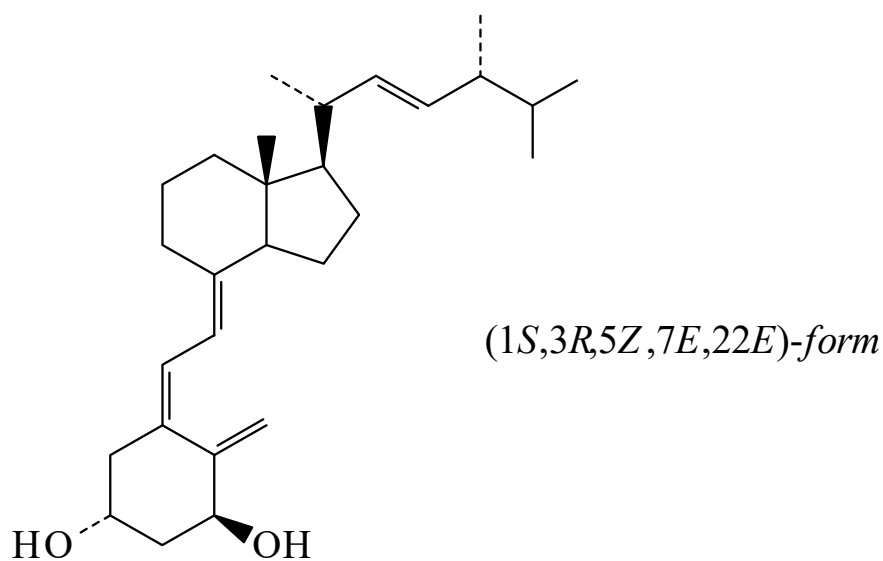




>>Entry Name: 9,10-Secoergosta-5,7,10(19),22-tetraene-1,3-diol, 9Cl



Related CAS Registry Numbers(s): 81126-34-3 81126-35-4

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.654

Accurate Mass: 412.33413

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Other Data: Deuterated compds. have been synth

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

Synonym(s): 5,6-*trans*-1 α -Hydroxyvitamin D₂

CAS Registry Number: 74007-20-8

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.654

Accurate Mass: 412.33413

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

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

Synonym(s): 1 α -Hydroxyvitamin D₂. **Doxercalciferol**, INN, USAN. Hectorol

CAS Registry Number: 54573-75-0

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.654

Accurate Mass: 412.33413

Percentage Composition: C 81.50%; H 10.75%; O 7.75%

Biological Use/Importance: Shows antileukaemic props. Stimulates Ca transport. Similar biol. activities to vitamin D₂

Physical Description: Cryst. (EtOAc/hexane)

Development Status: Launched 1999 (US)

Melting Point: Mp 141-143° (136-138°)

Optical Rotation: [α]_D²⁵+47.5 (c, 0.5 in EtOH)

Other Data: Pharmacol. active isomer

Hazard & Toxicity: LD₅₀ (rat, orl) 3.5 mg/kg

References:

- Lam, H.Y. *et al.*, *Steroids*, 1977, **30**, 671, (*synth*)
Paaren, H.E. *et al.*, *J.O.C.*, 1980, **45**, 3253, (*synth*)
Sjoeden, G. *et al.*, *J. Nutr.*, 1984, **114**, 2043, (*props*)
Andrews, D.R. *et al.*, *J.O.C.*, 1986, **51**, 1635, (*synth*)
Ostrem, V.K. *et al.*, *J. Biol. Chem.*, 1987, **262**, 14164, (*props*)
Tachibana, Y., *Bull. Chem. Soc. Jpn.*, 1988, **61**, 3915, (*synth*)
Perlman, K.L. *et al.*, *Chem. Comm.*, 1989, 1113, (*synth*)
Gallagher, J.C. *et al.*, *J. Bone Min. Res.*, 1994, **9**, 607, (*clin trial*)
Slatopolsky, E. *et al.*, *Kidney Int., Suppl.*, 1999, **73**, S14-S19; S59-S64