



>>Entry Name: 9,10-Secoergosta-5,7,10(19),22-tetraene-3,25-diol, 9Cl

Related CAS Registry Numbers(s): 79396-56-8 111422-22-1 111467-49-3 116405-15-3 116498-37-4 117467-29-5

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.654

Accurate Mass: 412.33413

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

Other Data: Tritiated compds. have been synth.

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

Synonym(s): 25-Hydroxyvitamin D₂. Ercalcidiol

CAS Registry Number: 21343-40-8

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.654

Accurate Mass: 412.33413

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

Source/Synthesis: Major metab. of vitamin D₂

Physical Description: Cryst. (hexane)

Melting Point: Mp 96-97°

Optical Rotation: [α]_D²⁵+56.8 (c, 0.2 in EtOH)

>>Derivative: 26,26,26,27,27,27-Hexafluoro deriv.

Synonym(s): 26,26,26,27,27,27-Hexafluoro-9,10-secoergosta-5,7,10(19),22-tetraene-3,25-diol, 9Cl

Molecular Formula: C₂₈H₃₈F₆O₂

Molecular Weight: 520.597

Accurate Mass: 520.277598

Percentage Composition: C 64.60%; H 7.36%; F 21.90%; O 6.15%

Use/Importance: Shows possible antileukaemic activity

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

Synonym(s): 24-*epi*-25-Hydroxyvitamin D₂

CAS Registry Number: 90191-28-9

Molecular Formula: C₂₈H₄₄O₂

Molecular Weight: 412.654

Accurate Mass: 412.33413

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

Optical Rotation: [α]_D²⁵+50.7 (c, 0.2 in EtOH)

References:

- Turnbull, H. *et al.*, *Clin. Chim. Acta*, 1982, **120**, 65, (*hplc*)
Morzycki, J.W. *et al.*, *J.O.C.*, 1984, **49**, 2148, (*synth, bibl*)
Yamada, S. *et al.*, *Tet. Lett.*, 1984, **25**, 3347, (*synth*)
Sardina, F.J. *et al.*, *J.O.C.*, 1986, **51**, 1264, (*synth, bibl*)
Synform, 1986, **4**, 131; 244, (*rev, synth*)
Koszewski, N.J. *et al.*, *Anal. Biochem.*, 1987, **162**, 446, (*pmr*)
Ostrem, V.K. *et al.*, *J. Biol. Chem.*, 1987, **262**, 14164, (*hexafluoro deriv*)
Mawer, E.B. *et al.*, *J. Chromatogr.*, 1987, **415**, 305, (*hplc*)
Castedo, L. *et al.*, *Tet. Lett.*, 1987, **28**, 4589, (*synth*)
Taguchi, T. *et al.*, *Tet. Lett.*, 1988, **29**, 227, (*synth, hexafluoro deriv*)
Coldwell, R.D. *et al.*, *Clin. Chim. Acta*, 1989, **180**, 157, (*gc-ms*)
Reddy, G.S. *et al.*, *Biochemistry*, 1990, **29**, 943, (*metab*)