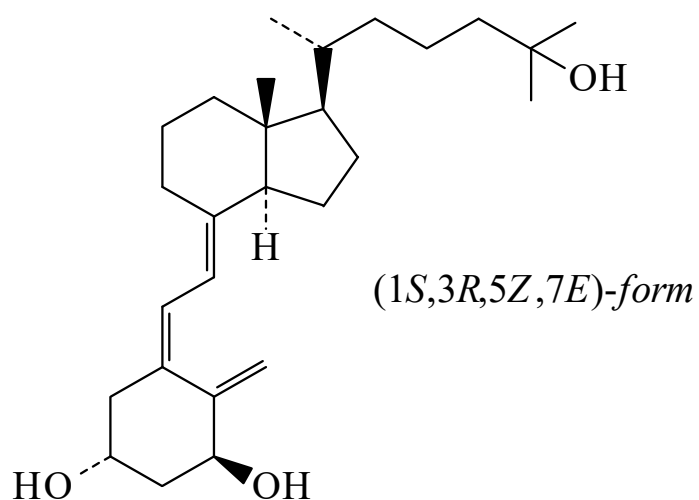




>>Entry Name: 9,10-Secocholesta-5,7,10(19)-triene-1,3,25-triol, 9Cl



Related CAS Registry Numbers(s): 32511-63-0 61476-45-7 66003-59-6 69254-35-9 72409-71-3 73890-65-0 74029-73-5 75917-61-2 76509-59-6 76509-60-9 77326-95-5 78782-99-7 80257-34-7 81126-40-1 81126-41-2 96614-28-7 96646-17-2 114906-52-4 120201-30-1 120328-18-9

Molecular Formula: C₂₇H₄₄O₃

Molecular Weight: 416.643

Accurate Mass: 416.329045

Percentage Composition: C 77.84%; H 10.64%; O 11.52%

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

CAS Registry Number: 73837-24-8

Molecular Formula: C₂₇H₄₄O₃

Molecular Weight: 416.643

Accurate Mass: 416.329045

Percentage Composition: C 77.84%; H 10.64%; O 11.52%

Melting Point: Mp 168-171°

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

Synonym(s): 1 α ,25-Dihydroxyvitamin D₃. 1 α ,25-Dihydroxycholecalciferol. **Calcitriol**, BAN, INN, USAN. Calcijex. Rocaltrol. Ro 21-5535. U 49562

CAS Registry Number: 32222-06-3

Molecular Formula: C₂₇H₄₄O₃

Molecular Weight: 416.643

Accurate Mass: 416.329045

Percentage Composition: C 77.84%; H 10.64%; O 11.52%

Biological Use/Importance: Used to treat vitamin D deficiency. Believed to be the hormonally active form of the vitamin. Calcium regulator. Has also been found to induce differentiation of certain myeloid and leukaemic cells. Used topically to treat psoriasis

Physical Description: Cryst. (methyl formate)

Development Status: Approved 1978

Melting Point: Mp 118-119°

Optical Rotation: [α]_D²⁵ +47.9 (c, 0.5 in EtOH)

Calculated Log P Data: Log P 5.18 (calc)

Sigma: D1530

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

CAS Registry Number: 66791-71-7

Molecular Formula: C₂₇H₄₄O₃

Molecular Weight: 416.643

Accurate Mass: 416.329045

Percentage Composition: C 77.84%; H 10.64%; O 11.52%

Physical Description: Oil

References: