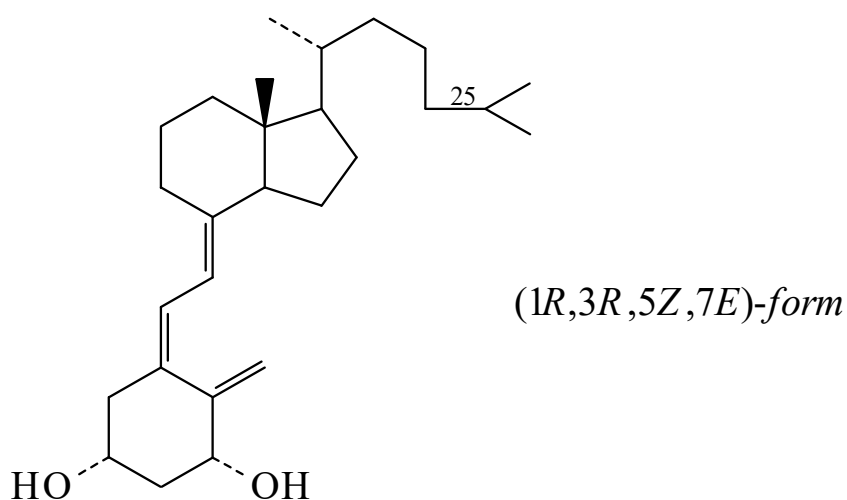




>>Entry Name: 9,10-Secocholesta-5,7,10(19)-triene-1,3-diol, 9Cl



Related CAS Registry Numbers(s): 58760-51-3 62073-74-9 69990-68-7 71726-09-5 71726-11-9 76135-93-8 80257-32-5 81126-22-9 81126-23-0 81126-24-1 89577-10-6 99956-42-0 99956-43-1

Molecular Formula: C₂₇H₄₄O₂

Molecular Weight: 400.643

Accurate Mass: 400.33413

Percentage Composition: C 80.94%; H 11.07%; O 7.99%

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

CAS Registry Number: 63181-13-5

Molecular Formula: C₂₇H₄₄O₂

Molecular Weight: 400.643

Accurate Mass: 400.33413

Percentage Composition: C 80.94%; H 11.07%; O 7.99%

Physical Description: Oil

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

CAS Registry Number: 65445-15-0

Molecular Formula: C₂₇H₄₄O₂

Molecular Weight: 400.643

Accurate Mass: 400.33413

Percentage Composition: C 80.94%; H 11.07%; O 7.99%

Physical Description: Oil

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

CAS Registry Number: 65445-14-9

Molecular Formula: C₂₇H₄₄O₂

Molecular Weight: 400.643

Accurate Mass: 400.33413

Percentage Composition: C 80.94%; H 11.07%; O 7.99%

Physical Description: Oil

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

Synonym(s): 1 α -Hydroxycholecalciferol. 1 α -Hydroxyvitamin D₃. **Alfacalcidol**, BAN, INN, JAN. Alfarol. Alpha D₃. α -Calcidiol. Dediol. Sinovul. EB 644

CAS Registry Number: 41294-56-8

Molecular Formula: C₂₇H₄₄O₂

Molecular Weight: 400.643

Accurate Mass: 400.33413

Percentage Composition: C 80.94%; H 11.07%; O 7.99%

Use/Importance: Used in treatment of vitamin D deficiency. Calcium regulator

Physical Description: Needles (Et₂O/petrol)

Melting Point: Mp 137-139°

Optical Rotation: [α]_D²⁰+28.9 (c, 0.28 in CHCl₃)

Calculated Log P Data: Log P 7.39 (uncertain value) (calc)

Other Data: Deuterated and tritiated compds. have been synthesised