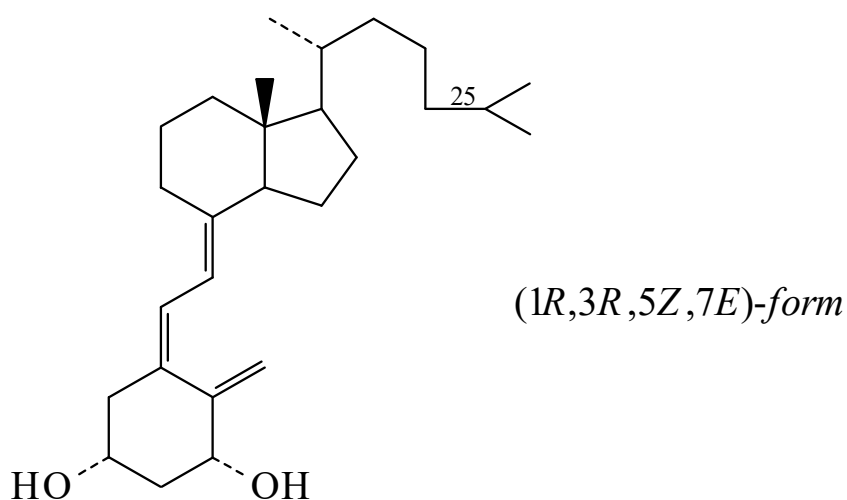




>>Entry Name: 9,10-Secocholesta-5,7,10(19)-triene-1,3-diol, 9Cl



**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:** C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>

**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:** C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>

**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:** C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>

**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:** C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>

**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 $\alpha$ -Hydroxycholecalciferol. 1 $\alpha$ -Hydroxyvitamin D<sub>3</sub>. **Alfacalcidol**, BAN, INN, JAN. Alfarol. Alpha D<sub>3</sub>.  $\alpha$ -Calcidiol. Dediol. Sinovul. EB 644

**CAS Registry Number:** 41294-56-8

**Molecular Formula:** C<sub>27</sub>H<sub>44</sub>O<sub>2</sub>

**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 (Et<sub>2</sub>O/petrol)

**Melting Point:** Mp 137-139°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>20</sup> +28.9 (c, 0.28 in CHCl<sub>3</sub>)

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

**Other Data:** Deuterated and tritiated compds. have been synthesised