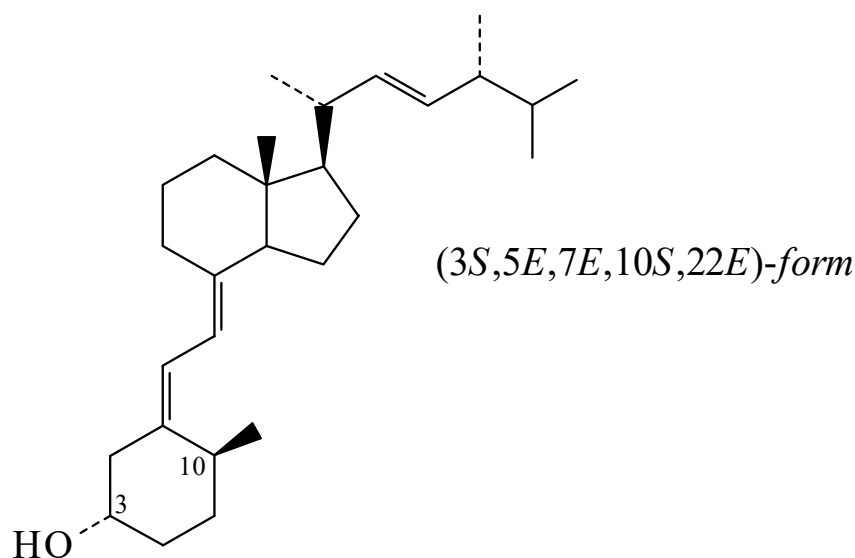




>>Entry Name: 9,10-Secoergosta-5,7,22-trien-3-ol, 9Cl



Related CAS Registry Numbers(s): 7665-90-9 83685-44-3 83685-45-4 85916-83-2 104846-64-2 104846-65-3 104874-69-3 104874-70-6

Molecular Formula: C₂₈H₄₆O

Molecular Weight: 398.671

Accurate Mass: 398.354865

Percentage Composition: C 84.36%; H 11.63%; O 4.01%

>>Variant: (3*R*,5*E*,7*E*,10*S*,22*E*)-form

CAS Registry Number: 62777-58-6

Molecular Formula: C₂₈H₄₆O

Molecular Weight: 398.671

Accurate Mass: 398.354865

Percentage Composition: C 84.36%; H 11.63%; O 4.01%

Physical Description: No phys. props. reported

>>Variant: (3*R*,5*Z*,7*E*,10*S*,22*E*)-form

CAS Registry Number: 116559-85-4

Molecular Formula: C₂₈H₄₆O

Molecular Weight: 398.671

Accurate Mass: 398.354865

Percentage Composition: C 84.36%; H 11.63%; O 4.01%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 111-113°

>>Variant: (3*R*,5*Z*,7*E*,10*R*,22*E*)-form

CAS Registry Number: 116559-86-5

Molecular Formula: C₂₈H₄₆O

Molecular Weight: 398.671

Accurate Mass: 398.354865

Percentage Composition: C 84.36%; H 11.63%; O 4.01%

Physical Description: Cryst. (Et₂O/hexane)

Melting Point: Mp 86-87°

>>Variant: (3*S*,5*E*,7*E*,10*S*,22*E*)-form

Synonym(s): Dihydrotachysterol, BAN, INN. Dihydrotachysterol₂. Antitetanin. Dichysterol. Hytakerol. Tachyrol

CAS Registry Number: 67-96-9

Molecular Formula: C₂₈H₄₆O

Molecular Weight: 398.671

Accurate Mass: 398.354865

Percentage Composition: C 84.36%; H 11.63%; O 4.01%

Use/Importance: Blood calcium regulator

Physical Description: Cryst. (MeOH)

Melting Point: Mp 131-132° (125-127°)

Optical Rotation: [α]_D²²+97.5 (CHCl₃)

Calculated Log P Data: Log P 9.85 (uncertain value) (calc)

Sigma: D9257