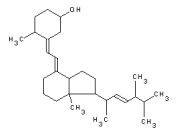

Formula: C28H46O

MW: 398.67

CAS: 67-96-9

TNP NUMBER: TNP00601

MDL NUMBER: MFCD09788229

IUPAC: 3-{2-[7-((2E)-1,4,5-trimethylhex-2-enyl)-6-methylbicyclo[4.3.0]non-2-ylidene]ethylidene}-4-methylcyclohexan-1-ol

Smiles: C1(=C/C=C2C3C(C(CC3)C(C=CC(C(C)C)C)C)(CCC2)C)/CC(CCC1C)O

Used to treat certain types of muscle cramps (tetany), regulates parathyroid hormone in persons with hypoparathyroidism

THERAPEUTIC CATEGORY: Calcium regulator

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 6

N+O: 1

Chiral Centers: 7

LogP: 11.41

LogS: -7.5

LIPINSKI: 3

Synonyms:
9,10-SECOERGOSTA-5,7,22-TRIEN-3BETA-OL;9,10-SECOERGOSTA-5,7,22-TRIEN-3B-OL;DICHYSTROLUM;DIHYDROTACHYSTEROL;CALCAMINE;AT-10;ANTITANIL;7,22-trien-3-ol,(3-beta,5e,7e,10-alpha,22e)-10-secoergosta-5

CAS:67-96-9

MF:C28H46O

MW:398.66

EINECS:200-672-7

Product Categories: DIHYDROTACHYSTEROL

Chemical Properties: storage temp. 2-8C Xn Risk Statements 22 Safety Statements 36 RIDADR UN 2811 6.1/PG 3 WGK Germany 3 RTECS WW0600000 HazardClass 6.1(b) PackingGroup III Hazardous Substances Data67-96-9(Hazardous Substances Data) DIHYDROTACHYSTEROL

Usage And Synthesis: DIHYDROTACHYSTEROL