



Formula: C₂₈H₄₄O

MW: 396.66

CAS: 57-87-4

TNP NUMBER: TNP00577

MDL NUMBER: MFCD07809368

IUPAC: 14-((2E)(1R,4R)-1,4,5-trimethylhex-2-enyl)(1S,5S,2R,11R,14R,15R)-2,15-dimethyl tetracyclo[8.7.0.0.0]heptadeca-7,9-dien-5-ol

Smiles:

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C1=2[C@H]3([C@]([C@@H]([C@@H](C=C[C@@H](C(C)C)C)CC3)(C)CC[C@@H]1([C]1(C)C[C@@H](CC1=CC2)O)C)
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Most important of the provitamines D. A crystalline sterol, C₂₈H₄₃OH, synthesized by yeast from sugars or derived from ergot and converted to vitamin D₂ when exposed to ultraviolet radiation

THERAPEUTIC CATEGORY: VITAMIN (Antirachitic)

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 4

N+O: 1

Chiral Centers: 8

LogP: 11.1

LogS: -7.37

LIPINSKI: 3

Synonyms:

(22E)-Ergosta-5,7,22-trien-3-ol;(22E,24R)-Ergosta-5,7,22-trien-3-ol;(3beta)-Ergosta-5,7,22-trien-3-ol;22-trien-3-ol,(3beta,22e)-ergosta-7;3-Hydroxy-(22E,24R)-ergosta-5,7,22-triene;7,22-trien-3-ol,(3.beta.)-Ergosta-5;delta-5,7,22-ergostatrien-3beta-ol;ergosta-5,7,22-trien-3beta-ol

CAS:57-87-4

MF:C28H44O

MW:396.65

EINECS:200-352-7

Product Categories:Pharmaceutical

Intermediates;Steroids;Biochemistry;Hydroxysteroids;Vitamins;Vitamins and derivatives
Ergosterol

Chemical Properties: mp 156-158 C(lit.) bp 250 C (1.3 mmHg) alpha -120 (c=1, CHCl3)
refractive index -112.5 (C=1, THF) storage temp. 2-8C Water Solubility PRACTICALLY
INSOLUBLE Sensitive Light Sensitive Merck 14,3659 Stability:Stable, but may be light or air
sensitive. Incompatible with acids, strong oxidizing agents.

CAS DataBase Reference: 57-87-4(

CAS DataBase Reference:) NIST Chemistry ReferenceErgosterol(57-87-4) T+,T Risk
Statements 28-48/20/22-40-38-25 Safety Statements 28-36/37-45 RIDADR UN 2811 6.1/PG 2
WGK Germany 3 F 1-3-8-10 HazardClass 6.1 PackingGroup II Hazardous Substances
Data57-87-4(Hazardous Substances Data) Provitamine D2 Ergosterol

Usage And Synthesis:

Chemical Properties: solid Ergosterol



