



Formula: C<sub>29</sub>H<sub>50</sub>O

MW: 414.72

CAS: 83-46-5

TNP NUMBER: TNP00383

MDL NUMBER: MFCD01821071

IUPAC: 14-((1S,4R)-4-ethyl-1,5-dimethylhexyl)(1S,5S,10S,11S,2R,14R,15R)-2,15-dimethyl tetracyclo[8.7.0.0.0]heptadec-7-en-5-ol

Smiles:

C12=CC[C@@H]3([C@@H]([C@@]1(C)CC[C@@H](C2)O)(CC[C]1(C)[C@H]3CC[C@@H]1[C@@H](CC[C@H](C(C)C)CC)C))

beta-Sitosterol, with ca. 10% campesterol, ca. 75% beta-sitosterol

THERAPEUTIC CATEGORY: Anticholesteremic. Treatment of prostaic adenoma

SOURCE: Common sterol in plants

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 4

N+O: 1

Chiral Centers: 9

LogP: 12.09

LogS: -7.77

LIPINSKI: 3

Synonyms:

B-SITOSTEROL;BETA-SITOSTEROL;A-PHYTOSTEROL;CINCHOL;22,23-DIHYDROSTIMASTEROL;22,23-DIHYDROSTIGMASTEROL;24-ALPHA-ETHYLCHOLESTEROL;24BETA-ETHYLCHOLESTEROL

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EINECS:201-480-6

Product Categories:Miscellaneous Natural

Products;Biochemistry;Hydroxysteroids;Steroids;Natural Plant Extract beta-Sitosterol

Chemical Properties: mp 136-140 C(lit.) alpha -28 (c=2, CHCl3) storage temp. -20C solubility chloroform: 20 mg/mL, clear, colorless Water Solubility INSOLUBLE Merck 8556

CAS DataBase Reference: 83-46-5(

CAS DataBase Reference: ) NIST Chemistry Reference