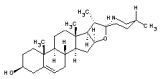

Formula: C27H43NO2

MW: 413.64

CAS: 126-17-0

TNP NUMBER: TNP00027

MDL NUMBER: MFCD09787895

IUPAC: (1S,2S,4S,7S,9S,12S,16S,8R,13R,26R)-7,9,13,23-tetramethyl-5-oxaspiro[pentacyclo[10.8.0.0.0.0]icosane-6,6'-piperidine]-18-en-16-ol

Smiles:
C=12[C](CC[C@@H](C2)O)([C@@H]2([C@@H](CC1)([C@H]1([C](CC2)([C@@H]2([C@H](C1)(O[C]1([C@H]2C)NCC(CC1)C)))C))))C

isolated from various Solanum species. Starting material for steroidal drugs

SOURCE: solated from various Solanum species. Starting material for steroidal drugs

ACCEPTORS: 2

DONORS: 2

ROTATION BONDS: 0

N+O: 3

Chiral Centers: 11

LogP: 8.71

LogS: -6.56

LIPINSKI: 3

Monograph Number: 0008783

Title: Solasodine

CAS Registry Number: 126-17-0

CAS Name: (3b,22a,25R)-Spirosol-5-en-3-ol

Additional Names: solasod-5-en-3b-ol; D5-20bF,22aF,25aF,27-azaspirosten-3b-ol; solancarpidine; solanidine-S; purapuridine

Molecular Formula: C27H43NO2

Molecular Weight: 413.64.

Percent Composition: C 78.40%, H 10.48%, N 3.39%, O 7.74%

Literature References: Steroidal alkaloid isolated from various Solanum species. By hydrolysis of solasonine: Rochelmeyer, Arch. Pharm. 277, 329 (1939). See also ref under Solasonine and Solanidine. Structure: Briggs et al., J. Chem. Soc. 1950, 3013. Synthesis: Uhle, J. Org. Chem. 27, 656 (1962); Schreiber, Ronsch, Tetrahedron 20, 1939 (1964); Kessar et al., ibid. 27, 2869 (1971). Comprehensive description: G. Indrayanto et al., Anal. Profiles Drug Subs. Excip. 24, 487-522 (1996).

Properties: Hexagonal plates from methanol or by sublimation in high vacuum, mp 200-202. [a]D25 -98 (c = 0.14 in methanol); [a]D -113 ($CHCl_3$). Alkaline reaction to litmus in alcoholic soln. pKb 6.30. uv max (methanol): 206 nm. Freely sol in benzene, pyridine, and chloroform. Practically insol in ether. Soly at 30 (mg/ml): methanol 9.5; 95% ethanol 5.0; acetone 3.5; n-hexane