



Formula: C<sub>25</sub>H<sub>42</sub>O<sub>4</sub>

MW: 406.61

CAS: 3245-38-3

MDL: MFCD00076102

TNP: TNP00438

METHYL DESOXYCHOLATE; METHYL DEOXYCHOLATE; DEOXYCHOLIC ACID METHYL ESTER; 5-BETA-CHOLAN-24-OIC ACID-3-ALPHA,12-ALPHA-DIOL METHYL ESTER; 5-BETA-CHOLANIC ACID-3-ALPHA, 12-ALPHA-DIOL METHYL ESTER; 3ALPHA,12ALPHA-DIHYDROXY-5BETA-CHOLAN-24-OIC ACID METHYL ESTER; deo



LogP: -2.53

LogS: -2.23

Acceptors: 4

Donors: 2

Rotation Bonds: 4

Chiral Centers: 10

N+O: 4

LIPINSKY: 4

IUPAC: methyl 4-((1S,2S,11S,16S,5R,7R,10R,14R,15R)-5,16-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0.0]heptadec-14-yl)pentanoate

Smiles:

C1[C@@H](CC[C]2([C@@H]1(CC[C@@H]1([C@@H]2(C[C@@H]([C]2([C@H]1(CC[C@@H]

2([C@H](C)CCC(OC)=O))C)O)))C)O

Specification: Steroids & Hormones - 13C & 2H; Steroids METHYL DESOXYCHOLATE

METHYL DESOXYCHOLATE Usage And Synthesis Chemical Properties:

White Crystalline Solid METHYL DESOXYCHOLATE