



Formula: C<sub>25</sub>H<sub>42</sub>O<sub>5</sub>

MW: 422.61

CAS: 1448-36-8

MDL: MFCD00477541

TNP: TNP00413

5(BETA)-CHOLAMIC ACID-3ALPHA,7ALPHA,12ALPHA-TRIOL METHYL ESTER;  
5-BETA-CHOLANIC ACID-3-ALPHA, 7-ALPHA, 12-ALPHA-TRIOL METHYL ESTER; METHYL  
4-(3,7,12-TRIHYDROXY-10,13-DIMETHYLPERHYDROCYCLOPENTA[A]PHENANTHREN-17-  
YL)PENTANOATE; METHYL CHOLATE; CHOLIC ACID METHYL



LogP: 4.02

LogS: -4.79

Acceptors: 5

Donors: 3

Rotation Bonds: 5

Chiral Centers: 11

N+O: 5

LIPINSKY: 4

IUPAC: methyl 4-(((16S,5R,9R)-5,9,16-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0.0  
]heptadec-14-yl)pentanoate

Smiles:

C1C2C3(C(C[C@@H](CC3)O)C[C@H](C2C2C([C@H]1O)(C(CC2)C(CCC(=O)OC)C)C)O)C

Specification: Steroids; Steroids & Hormones - 13C & 2H CHOLIC ACID METHYL ESTER  
Chemical Properties:

mp 155-156C Merck 14,2203 BRN 2226989 CAS DataBase Reference 1448-36-8 (CAS  
DataBase Reference) Safety Information Hazard Codes Xi Safety Statements 22-24/25  
CHOLIC ACID METHYL ESTER Usage And Synthesis Chemical Properties:

Off-White Solid CHOLIC ACID METHYL ESTER Preparation Products Ursodeoxycholic acid