



Formula: C₂₄H₄₀O₄

MW: 392.58

CAS: 128-13-2

MDL NUMBER: MFCD00066760

IUPAC: 4-(5,9-dihydroxy-2,15-dimethyltetracyclo[8.7.0.0.0]heptadec-14-yl) pentanoic acid

Smiles: C1C2(C(C3C(CC4C(C3C1)(CCC(O)C4)C)O)CCC2C(CCC(=O)O)C)C

Found in bear bile

THERAPEUTIC CATEGORY: Anticholelithogenic

ACCEPTORS: 4

DONORS: 3

ROTATION BONDS: 7

N+O: 4

Chiral Centers: 10

LogP: 7.09

LogS: -5.79

LIPINSKI: 3

Synonyms: 7BETA-HYDROXYLITHOCHOLIC ACID;6BETA-CHOLANIC ACID-3A,7BETA-DIOL;(6-BETA)-CHOLANIC ACID-(3-ALPHA)-(7-BETA)-DIOL;3A,7B-DIHYDROXY-5B-CHOLAN-24-OIC ACID;3ALPHA, 7BETA-DIHYDROXY-5BETA-CHOLANIC ACID;3ALPHA,7BETA-DIHYDROXY-5BETA-CHOLAN-24-OIC ACID;3alpha,7beta-dihydroxy-6beta-cholan-24-oic acid;3ALPHA, 7BETA-DIOXYCHOLANIC ACID

CAS:128-13-2

MF:C24H40O4

MW:392.57

EINECS:204-879-3

Product Categories:Bile Acids;Biochemistry;Steroids;Intermediates & Fine Chemicals;Pharmaceuticals;API's Ursodeoxycholic acid

Chemical Properties: mp 203-204 C(lit.) alpha 60 (c=2, EtOH) refractive index 60.5 (C=2, EtOH) solubility ethanol: 50 mg/mL, clear Water Solubility practically insoluble Merck 14,9889

CAS DataBase Reference: 128-13-2(

CAS DataBase Reference:) Xi Risk Statements 36/37/38 Safety Statements 24/25-36-26 WGK Germany 2 RTECS FZ2000000 F 10 3alpha,7beta-Dihydroxy-6beta-cholan-24-oic acid Ursodeoxycholic acid

Usage And Synthesis:

Chemical Properties: WHITE CRYSTALLINE POWDER UsageUsed as an anticholelithogenic Ursodeoxycholic acid

