



Formula: C₂₄H₃₄O₅

MW: 402.53

CAS: 81-23-2

TNP NUMBER: TNP00592

MDL NUMBER: MFCD03225547

IUPAC: 4-((1S,2S,7S,11S,10R,14R,15R)-2,15-dimethyl-5,9,16-trioxotetracyclo[8.7.0.0<2,7>.0<11,15>]heptadec-14-yl)pentanoic acid

Smiles:

C(=O)(O)CC[C@@H](C)[C@@H]1[C]2([C@H]([C@@H]3(C(C[C@H]4([C]([C@H]3(CC2=O))(C CC(C4)=O)C))=O))(CC1))C

THERAPEUTIC CATEGORY: Choleric

ACCEPTORS: 5

DONORS: 1

ROTATION BONDS: 4

N+O: 5

Chiral Centers: 8

LogP: 4.32

LogS: -5.08

LIPINSKI: 4

Synonyms: TRIKETOCHOLANIC;KETOCHOLANIC ACID;DEHYDROCHOLIC ACID;5BETA-CHOLANIC ACID-3,5,12-TRIONE;5-BETA-CHOLANIC ACID-3,7,12-TRIONE;3,7,12-TRIOXO-5B-CHOLENE-24-OIC ACID;3,7,12-TRIOXO-5-BETA-CHOLAMIC ACID;3,7,12-TRIOXO-5BETA-CHOLAN-24-OIC ACID

CAS:81-23-2

MF:C24H34O5

MW:402.52

EINECS:201-335-7

Product Categories:Bile Acids;Biochemistry;Steroids Dehydrocholic acid

Chemical Properties: mp 238-240 C alpha 29 (c=2, dioxane) refractive index 30.5 (C=2, Dioxane) solubility ethanol: 10 mg/mL Merck 14,2868 BRN 3226734

CAS DataBase Reference: 81-23-2(

CAS DataBase Reference:) NIST Chemistry Reference Dehydrocholic acid(81-23-2) EPA
Substance Registry System Cholan-24-oic acid, 3,7,12-trioxo-, (5.beta.)-(81-23-2)

Safety Information: Safety Statements 24/25 WGK Germany 2 RTECS FZ2300000
3,7,12-Trioxo-5beta-cholan-24-oic acid Dehydrocholic acid

Usage And Synthesis:

Chemical Properties: white to off-white amorphous powder Dehydrocholic acid

