



Formula: C<sub>24</sub>H<sub>40</sub>O<sub>3</sub>

MW: 376.58

CAS: 434-13-9

MDL: MFCD03225520

TNP: TNP00406

3-HYDROXYCHOLANIC ACID; 3ALPHA-HYDROXYCHOLANIC ACID;  
3ALPHA-HYDROXY-5BETA-CHOLANIC ACID; 3ALPHA-HYDROXY-5BETA-CHOLAN-24-OIC  
ACID; 5BETA-CHOLAN-24-OIC ACID-3A-OL; 5BETA-CHOLAN-24-OIC ACID-3ALPHA-OL;  
5BETA-CHOLANIC ACID-3ALPHA-OL; LITHOCHOLIC ACID



LogP: -1.67

LogS: -1.88

Acceptors: 3

Donors: 2

Rotation Bonds: 4

Chiral Centers: 9

N+O: 3

LIPINSKY: 4

Info: Lithocholic acid 98%

IUPAC: (4S)-4-(((1S,2S,11S,5R,7R,10R,14R,15R)-5-hydroxy-2,15-dimethyltetracyclo[8.7.0.0.0]heptadec-14-yl)pentanoic acid

Smiles:

C1[C@H]2([C@@H]([C@@H]3(CC[C@H]4([C]([C@@H]3(C1)))(CC[C@H](O)C4)C)))(CC[C@@H]2[C@@H](CCC(=O)O)C)C

Specification: Steroids; Bile Acids; Biochemistry LITHOCHOLIC ACID Chemical Properties:

mp 183-188 C(lit.) refractive index 35.5 (C=1, EtOH) Merck 5545 CAS DataBase Reference434-13-9(CAS DataBase Reference) Safety 22-24/25 WGK Germany 2 RTECS FZ2275000LITHOCHOLIC ACID Usage And Synthesis Chemical Properties:

white to off-white powder General DescriptionHexagonal leaflets (from alcohols) or prisms (from acetic acid) or white powder. Air & Water ReactionsInsoluble in water. Health HazardACUTE/CHRONIC HAZARDS: When heated to decomposition LITHOCHOLIC ACID emits acrid smoke and fumes. Fire HazardFlash point data for LITHOCHOLIC ACID are not available. LITHOCHOLIC ACID is probably combustible. LITHOCHOLIC ACID

Merck 13 Reference: Monograph Number: 0005565

Title: Lithocholic Acid

CAS Registry Number: 434-13-9

CAS Name: (3a,5b)-3-Hydroxycholan-24-oic acid

Additional Names: 3a-hydroxycholanic acid; 17b-(1-methyl-3-carboxypropyl)etiocholan-3a-ol

Molecular Formula: C<sub>24</sub>H<sub>40</sub>O<sub>3</sub>

Molecular Weight: 376.57.

Percent Composition: C 76.55%, H 10.71%, O 12.75%

Literature References: Found in ox bile, human bile, rabbit bile, and in ox and pig gallstones. Isoln: Fischer, Z. Physiol. Chem. 73, 234 (1911). Characterization: Wieland, Weyland, *ibid.* 110, 123 (1920). Prepn from cholic or from desoxycholic acid: Hoehn, Mason, J. Am. Chem. Soc. 62, 569 (1940); Sarel, Yanuka, J. Org. Chem. 24, 2018 (1959). Crystal and molecular structure by x-ray diffraction: S. K. Arora et al., *Acta Crystallogr.* 32B, 415 (1976).

Properties: Hexagonal leaflets from alcohol, prisms from acetic acid, mp 184-186. [α]<sub>D</sub><sup>20</sup> +33.7 (c = 1.5 in abs ethanol); [α]<sub>D</sub><sup>19</sup> +23.3 (Wieland); [α]<sub>D</sub><sup>20</sup> +32.1 (Fischer). Freely sol in hot alc. More sol in ether than cholic or desoxycholic acid. Sol in about 10 times its weight of ethyl acetate. Slightly sol in glacial acetic acid (about 0.2 g in 3 ml). More sol in benzene than desoxycholic acid. Insol in petr ether, gasoline, ligroin, water.

Melting point: mp 184-186

Optical Rotation:  $[\alpha]_{D20} +33.7$  ( $c = 1.5$  in abs ethanol);  $[\alpha]_{D19} +23.3$  (Wieland);  $[\alpha]_{D20} +32.1$  (Fischer)

Derivative Type: Methyl ester

Molecular Formula:  $C_{25}H_{42}O_3$

Molecular Weight: 390.60.

Percent Composition: C 76.87%, H 10.84%, O 12.29%

Properties: Crystallizes with