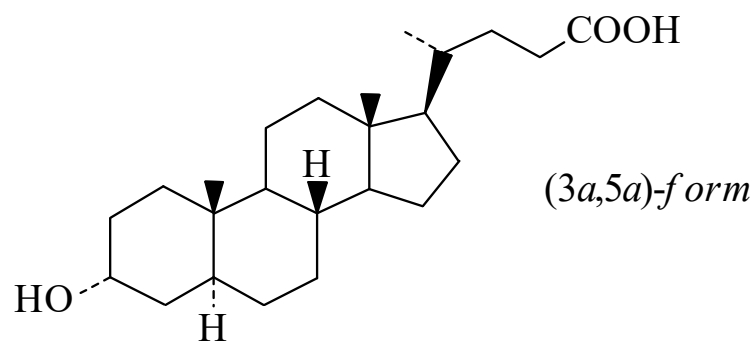




>>Entry Name: 3-Hydroxycholan-24-oic acid

ENTRY UNDER REVIEW

Synonym(s): 3-Hydroxycholanic acid



CAS Registry Number: 35498-67-0

Molecular Formula: C₂₄H₄₀O₃

Molecular Weight: 376.578

Accurate Mass: 376.297745

Percentage Composition: C 76.55%; H 10.71%; O 12.75%

>>Variant: (3 α ,5 α)-form

Synonym(s): Allolithocholic acid

CAS Registry Number: 2276-94-0

Molecular Formula: C₂₄H₄₀O₃

Molecular Weight: 376.578

Accurate Mass: 376.297745

Percentage Composition: C 76.55%; H 10.71%; O 12.75%

Biological Source: Isol. from human faeces

Melting Point: Mp 204-208°

Optical Rotation: $[\alpha]_D^{26} +26$

>>Derivative: Me ester

CAS Registry Number: 15074-01-8

Molecular Formula: C₂₅H₄₂O₃

Molecular Weight: 390.605

Accurate Mass: 390.313395

Percentage Composition: C 76.87%; H 10.84%; O 12.29%

Melting Point: Mp 160-161°

>>Variant: (3 α ,5 β)-form

Synonym(s): Lithocholic acid

CAS Registry Number: 434-13-9

Molecular Formula: C₂₄H₄₀O₃

Molecular Weight: 376.578

Accurate Mass: 376.297745

Percentage Composition: C 76.55%; H 10.71%; O 12.75%

Biological Source: Occurs in human, cattle and rabbit bile, and in cattle and pig gallstones. A major secondary, faecal, bile acid

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 186°

Optical Rotation: $[\alpha]_D^{20} +33.7$ (c, 1.5 in EtOH)

UV: [neutral] $\lambda_{\max}$ (EtOH) (Berdy)

Hazard & Toxicity: Exp. reprod. and teratogenic effects. LD₅₀ (mus, orl) 3900 mg/kg

Aldrich: 86006-9

Fluka: 62620

Sigma: L6250

>>Derivative: Me ester

CAS Registry Number: 1249-75-8

Physical Description: Cryst. (MeOH)

Melting Point: Mp 90-93°. Mp 130° (dimorph.)

Sigma: L6507