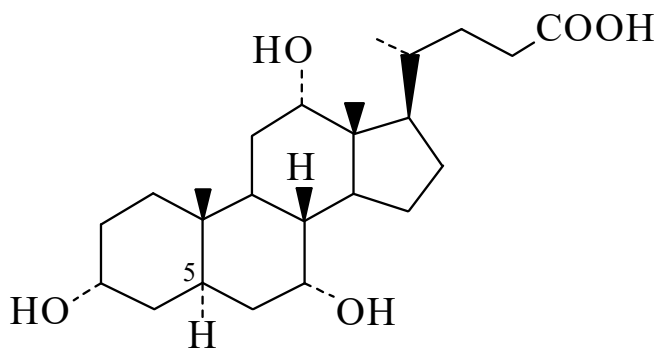




>>Entry Name: 3,7,12-Trihydroxycholan-24-oic acid



Related CAS Registry Numbers(s): 361-09-1

Molecular Formula: C₂₄H₄₀O₅

Molecular Weight: 408.577

Accurate Mass: 408.287575

Percentage Composition: C 70.55%; H 9.87%; O 19.58%

>>Variant: (3 α ,5 α ,7 α ,12 α)-form

Synonym(s): Allocholic acid

CAS Registry Number: 2464-18-8

Molecular Formula: C₂₄H₄₀O₅

Molecular Weight: 408.577

Accurate Mass: 408.287575

Percentage Composition: C 70.55%; H 9.87%; O 19.58%

Biological Source: Isol. from many animal sources. Bile acid in penguin (*Pinguinus impennis*) and sturgeon (*Acipenser sturio*)

Physical Description: Cryst. (Me₂CO aq.)

Melting Point: Mp 250-251°

Optical Rotation: [α]_D²⁵+27.8 (c, 0.75 in MeOH)

>>Derivative: Me ester

CAS Registry Number: 861-83-6

Molecular Formula: C₂₅H₄₂O₅

Molecular Weight: 422.604

Accurate Mass: 422.303225

Percentage Composition: C 71.05%; H 10.02%; O 18.93%

Physical Description: Cryst. (Me₂CO/hexane)

Melting Point: Mp 225-226°

Optical Rotation: [α]_D²⁵+26.7 (c, 0.84 in MeOH)

>>Variant: (3 α ,5 β ,7 α ,12 α)-form

Synonym(s): Cholic acid. Cholalic acid. Cholagit. Colalin. Hypocholate. NSC 6135

CAS Registry Number: 81-25-4

Molecular Formula: C₂₄H₄₀O₅

Molecular Weight: 408.577

Accurate Mass: 408.287575

Percentage Composition: C 70.55%; H 9.87%; O 19.58%

Biological Source: Isol. from bile and animal excretions. Widespread primary bile acid found in many spp.

Use/Importance: Choleric, laxative. Forms many inclusion complexes, has been used as a resolving agent

Physical Description: Cryst. + 1 H₂O (H₂O or Et₂O aq.). Cryst. + 1EtOH (EtOH)

Melting Point: Mp 197° (anhyd.)

Optical Rotation: [α]_D²⁰+37 (EtOH)

pKa Value: pK_{a1} 4.98 (20°)

Calculated Log P Data: Log P 2.39 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 4950 mg/kg

Aldrich: 13524-0

Fluka: 27010

Sigma: C1129