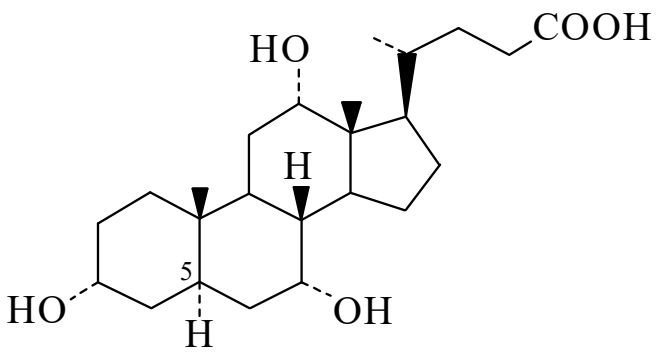
>>**Entry Name: 3,7,12-Trihydroxycholan-24-oic acid**



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

Molecular Formula: $C_{24}H_{40}O_5$
Molecular Weight: 408.577
Accurate Mass: 408.287575
Percentage Composition: C 70.55%; H 9.87%; O 19.58%

>>**Variant:** (3α,5α,7α,12α)-form
Synonym(s): Allocholic acid

CAS Registry Number: 2464-18-8

Molecular Formula: $C_{24}H_{40}O_5$
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. (Me_2CO aq.)
Melting Point: Mp 250-251°
Optical Rotation: $[\alpha]_D^{25}$+27.8 (c, 0.75 in MeOH)

>>**Derivative:** Me ester

CAS Registry Number: 861-83-6
Molecular Formula: $C_{25}H_{42}O_5$
Molecular Weight: 422.604
Accurate Mass: 422.303225
Percentage Composition: C 71.05%; H 10.02%; O 18.93%
Physical Description: Cryst. (Me_2CO/hexane)
Melting Point: Mp 225-226°
Optical Rotation: $[\alpha]_D^{25}$+26.7 (c, 0.84 in MeOH)

>>**Variant:** (3α,5β,7α,12α)-form
Synonym(s): Cholic acid. Cholalic acid. Cholagit. Colalin. Hypocholate. NSC 6135

CAS Registry Number: 81-25-4

Molecular Formula: $C_{24}H_{40}O_5$
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: Choleretic, laxative. Forms many inclusion complexes, has been used as a resolving agent
Physical Description: Cryst. + 1 H_2O (H_2O or Et_2O aq.). Cryst. + 1EtOH (EtOH)
Melting Point: Mp 197° (anhyd.)
Optical Rotation: $[\alpha]_D^{20}$+37 (EtOH)
pKa Value: pK_{a1} 4.98 (20°)
Calculated Log P Data: Log P 2.39 (uncertain value) (calc)
Hazard & Toxicity: LD_{50} (mus, orl) 4950 mg/kg

Aldrich: 13524-0
Fluka: 27010
Sigma: C1129