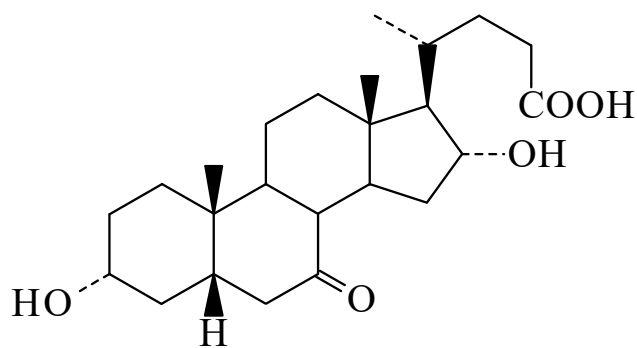




>>Entry Name: 3-Hydroxy-7-oxocholan-24-oic acid



Molecular Formula: C₂₄H₃₈O₄

Molecular Weight: 390.562

Accurate Mass: 390.27701

Percentage Composition: C 73.81%; H 9.81%; O 16.39%

>>Variant: (3 α ,5 β)-form

Synonym(s): Nutriacholic acid. Cavicholic acid. 7-Ketolithocholic acid

CAS Registry Number: 4651-67-6

Molecular Formula: C₂₄H₃₈O₄

Molecular Weight: 390.562

Accurate Mass: 390.27701

Percentage Composition: C 73.81%; H 9.81%; O 16.39%

Biological Source: Oxidn. product of chenodeoxycholic acid. Isol. from bile and faeces

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 203-204°

Optical Rotation: [α]_D -26 (c, 0.1 in MeOH)

>>Derivative: Me ester

CAS Registry Number: 10538-59-7

Molecular Formula: C₂₅H₄₀O₄

Molecular Weight: 404.589

Accurate Mass: 404.29266

Percentage Composition: C 74.22%; H 9.96%; O 15.82%

Melting Point: Mp 107-109°

Optical Rotation: [α]_D²⁰ -38 (c, 1.63 in CHCl₃)

>>Derivative: Me ester, Ac

Molecular Formula: C₂₇H₄₂O₅

Molecular Weight: 446.626

Accurate Mass: 446.303225

Percentage Composition: C 72.61%; H 9.48%; O 17.91%

Melting Point: Mp 145-148°

Optical Rotation: [α]_D¹⁹ -1 (c, 1.51 in CHCl₃)

>>Derivative: Glycine amide

Synonym(s): N-(3-Hydroxy-7-oxocholan-24-oyl) glycine

Molecular Formula: C₂₆H₄₁NO₅

Molecular Weight: 447.614

Accurate Mass: 447.298474

Percentage Composition: C 69.77%; H 9.23%; N 3.13%; O 17.87%

Melting Point: Mp 179-181°