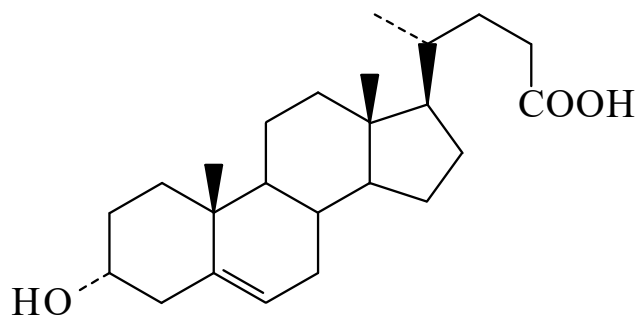




>>Entry Name: 3-Hydroxychol-5-en-24-oic acid

Synonym(s): 3-Hydroxychol-5-enic acid



Molecular Formula: C₂₄H₃₈O₃

Molecular Weight: 374.562

Accurate Mass: 374.282095

Percentage Composition: C 76.96%; H 10.23%; O 12.81%

>>Variant: 3 α -form

CAS Registry Number: 474-57-7

Molecular Formula: C₂₄H₃₈O₃

Molecular Weight: 374.562

Accurate Mass: 374.282095

Percentage Composition: C 76.96%; H 10.23%; O 12.81%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 199-200°

Optical Rotation: [α]_D²¹ -25.5 (c, 1 in CHCl₃)

>>Derivative: Me ester

CAS Registry Number: 14956-24-2

Molecular Formula: C₂₅H₄₀O₃

Molecular Weight: 388.589

Accurate Mass: 388.297745

Percentage Composition: C 77.27%; H 10.37%; O 12.35%

Melting Point: Mp 127°

Optical Rotation: [α]_D²¹ -30 (c, 1 in CHCl₃)

>>Derivative: Me ester, Ac

CAS Registry Number: 3633-72-5

Molecular Formula: C₂₇H₄₂O₄

Molecular Weight: 430.626

Accurate Mass: 430.30831

Percentage Composition: C 75.31%; H 9.83%; O 14.86%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 109-111°

Optical Rotation: [α]_D²¹ -18.5 (c, 1 in CHCl₃)

>>Variant: 3 β -form

CAS Registry Number: 5255-17-4

Molecular Formula: C₂₄H₃₈O₃

Molecular Weight: 374.562

Accurate Mass: 374.282095

Percentage Composition: C 76.96%; H 10.23%; O 12.81%

Physical Description: Needles (EtOAc or MeOH aq.)

Melting Point: Mp 240-242° (218-221°)

Optical Rotation: [α]_D²⁰ -36 (c, 0.116 in EtOH)

Sigma: C2650

>>Derivative: Me ester

CAS Registry Number: 20231-57-6

Physical Description: Needles (CH₂Cl₂/hexane)

Melting Point: Mp 147-148.5°

Optical Rotation: [α]_D -39.6 (c, 1 in CHCl₃)

Sigma: H5511