



>>Entry Name: Cholest-4-en-3-ol, 9CI

Molecular Formula: C₂₇H₄₆O

Molecular Weight: 386.66

Accurate Mass: 386.354865

Percentage Composition: C 83.87%; H 11.99%; O 4.14%

>>Variant: 3 α -form

Synonym(s): Epiallocholesterol

CAS Registry Number: 566-90-5

Molecular Formula: C₂₇H₄₆O

Molecular Weight: 386.66

Accurate Mass: 386.354865

Percentage Composition: C 83.87%; H 11.99%; O 4.14%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 83-84°

Optical Rotation: [α]_D²⁵+119 (c, 1 in CHCl₃)

>>Derivative: Ac

CAS Registry Number: 63730-40-5

Molecular Formula: C₂₉H₄₈O₂

Molecular Weight: 428.697

Accurate Mass: 428.36543

Percentage Composition: C 81.25%; H 11.29%; O 7.46%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 83-84°

Optical Rotation: [α]_D+177 (c, 1.0 in CHCl₃)

>>Derivative: Me ether

Synonym(s): 3-Methoxycholest-4-ene

CAS Registry Number: 17320-23-9

Molecular Formula: C₂₈H₄₈O

Molecular Weight: 400.687

Accurate Mass: 400.370515

Percentage Composition: C 83.93%; H 12.07%; O 3.99%

Physical Description: Cryst. (Me₂CO/MeOH)

Melting Point: Mp 45-46°

Optical Rotation: [α]_D+70 (c, 1.0 in CHCl₃)

>>Variant: 3 β -form

Synonym(s): Allocholesterol

CAS Registry Number: 517-10-2

Molecular Formula: C₂₇H₄₆O

Molecular Weight: 386.66

Accurate Mass: 386.354865

Percentage Composition: C 83.87%; H 11.99%; O 4.14%

Physical Description: Needles (EtOH)

Melting Point: Mp 132-134°

Optical Rotation: [α]_D+53 (CHCl₃)

>>Derivative: Ac

CAS Registry Number: 4087-12-1

Molecular Formula: C₂₉H₄₈O₂

Molecular Weight: 428.697

Accurate Mass: 428.36543

Percentage Composition: C 81.25%; H 11.29%; O 7.46%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 87-88°

Optical Rotation: [α]_D+10 (c, 1.8 in CHCl₃)