



>>Entry Name: Cholest-5-ene-3,25-diol, 9Cl

Molecular Formula: C₂₇H₄₆O₂

Molecular Weight: 402.659

Accurate Mass: 402.34978

Percentage Composition: C 80.54%; H 11.51%; O 7.95%

>>Variant: 3 α -form

Molecular Formula: C₂₇H₄₆O₂

Molecular Weight: 402.659

Accurate Mass: 402.34978

Percentage Composition: C 80.54%; H 11.51%; O 7.95%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 156-157°

Optical Rotation: [α]_D²⁸ -41.5 (CHCl₃)

>>Derivative: 3-Ac

CAS Registry Number: 67371-50-0

Molecular Formula: C₂₉H₄₈O₃

Molecular Weight: 444.696

Accurate Mass: 444.360345

Percentage Composition: C 78.33%; H 10.88%; O 10.79%

Physical Description: Oil

>>Variant: 3 β -form

Synonym(s): 25-Hydroxycholesterol

CAS Registry Number: 2140-46-7

Molecular Formula: C₂₇H₄₆O₂

Molecular Weight: 402.659

Accurate Mass: 402.34978

Percentage Composition: C 80.54%; H 11.51%; O 7.95%

Physical Description: Needles (MeOH)

Melting Point: Mp 179-181°

Optical Rotation: [α]_D²⁵ -39 (c, 1.05 in CHCl₃)

Fluka: 55125

Sigma: H1015

>>Derivative: 3-Ac

CAS Registry Number: 10525-22-1

Molecular Formula: C₂₉H₄₈O₃

Molecular Weight: 444.696

Accurate Mass: 444.360345

Percentage Composition: C 78.33%; H 10.88%; O 10.79%

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 139-140°

Optical Rotation: [α]_D²⁵ -41.4 (c, 1.05 in CHCl₃)

>>Derivative: Di-Ac

CAS Registry Number: 59975-17-6

Molecular Formula: C₃₁H₅₀O₄

Molecular Weight: 486.734

Accurate Mass: 486.37091

Percentage Composition: C 76.50%; H 10.35%; O 13.15%

Physical Description: Plates (MeOH)

Melting Point: Mp 119-120°