



>>Entry Name: Cholest-5-ene-3,20-diol, 9Cl
ENTRY UNDER REVIEW

CAS Registry Number: 29913-75-5

Molecular Formula: C₂₇H₄₆O₂
Molecular Weight: 402.659
Accurate Mass: 402.34978
Percentage Composition: C 80.54%; H 11.51%; O 7.95%

>>Variant: (3β,20*R*)-form
Synonym(s): 3β,20β-form

CAS Registry Number: 7484-22-2

Molecular Formula: C₂₇H₄₆O₂
Molecular Weight: 402.659
Accurate Mass: 402.34978
Percentage Composition: C 80.54%; H 11.51%; O 7.95%
Melting Point: Mp 115-117°
Optical Rotation: [α]_D −61 (CHCl₃)

>>Derivative: 3-Ac

CAS Registry Number: 7429-99-4
Molecular Formula: C₂₉H₄₈O₃
Molecular Weight: 444.696
Accurate Mass: 444.360345
Percentage Composition: C 78.33%; H 10.88%; O 10.79%
Melting Point: Mp 113-114°
Optical Rotation: [α]_D −47 (CHCl₃)

>>Variant: (3β,20*S*)-form
Synonym(s): 3β,20α-form

CAS Registry Number: 516-72-3

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. (heptane)
Melting Point: Mp 136-137°
Optical Rotation: [α]_D −57 (CHCl₃)
Aldrich: 28612-5
Sigma: H6378

>>Derivative: 3-Ac

CAS Registry Number: 7484-20-0
Physical Description: Cryst. (MeOH)
Melting Point: Mp 156-157° (135°)
Optical Rotation: [α]_D −59 (CHCl₃)

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **3**, 568B, (*nmr*)
Mijares, A. *et al.*, *J.O.C.*, 1967, **32**, 810, (*synth*)
Velgová, H. *et al.*, *Coll. Czech. Chem. Comm.*, 1969, **34**, 3354, (*synth*, 3β,20*S*-form)
van Lier, J.E. *et al.*, *J.O.C.*, 1970, **35**, 2627, (*synth*, *ir*, 3β,20*S*-form)
Sheikh, Y.M. *et al.*, *J.O.C.*, 1973, **38**, 3545, (*synth*, *pmr*, 3β-form)
Lin, Y.Y., *Lipids*, 1980, **15**, 756, (*ms*, 3β-form)