



>>Entry Name: Cholest-5-ene-3,26-diol, 9Cl

Related CAS Registry Numbers(s): 56792-58-6 56845-81-9

Molecular Formula:  $C_{27}H_{46}O_2$

Molecular Weight: 402.659

Accurate Mass: 402.34978

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

>>Variant: (3 $\beta$ ,25*R*)-form

Synonym(s): (25*R*)-26-Hydroxycholesterol

CAS Registry Number: 20380-11-4

Extra CAS Registry Numbers(s): 13095-61-9

Molecular Formula:  $C_{27}H_{46}O_2$

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 177-178°

Optical Rotation:  $[\alpha]_D^{24}$  -40.6 (c, 1.277 in  $CHCl_3$ )

>>Derivative: Di-Ac

Molecular Formula:  $C_{31}H_{50}O_4$

Molecular Weight: 486.734

Accurate Mass: 486.37091

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

Physical Description: Cryst. (MeOH)

Melting Point: Mp 128-129°

Optical Rotation:  $[\alpha]_D^{20}$  -37 (c, 0.9 in  $CHCl_3$ )

>>Variant: (3 $\beta$ ,25*S*)-form

Synonym(s): (25*S*)-26-Hydroxycholesterol

CAS Registry Number: 56845-83-1

Extra CAS Registry Numbers(s): 13095-61-9

Molecular Formula:  $C_{27}H_{46}O_2$

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 177-178°

Optical Rotation:  $[\alpha]_D^{23}$  -44 (c, 1.00 in  $CHCl_3$ )

>>Derivative: 3-Ac

CAS Registry Number: 113974-74-6

Molecular Formula:  $C_{29}H_{48}O_3$

Molecular Weight: 444.696

Accurate Mass: 444.360345

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

Physical Description: Cryst. (MeOH)

Melting Point: Mp 132-133°

Optical Rotation:  $[\alpha]_D^{25}$  -46.6 (c, 1.00 in  $CHCl_3$ )

>>Derivative: Di-Ac

CAS Registry Number: 66964-90-7

Molecular Formula:  $C_{31}H_{50}O_4$

Molecular Weight: 486.734

Accurate Mass: 486.37091

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

Melting Point: Mp 99-100°

Optical Rotation:  $[\alpha]_D^{20}$  -34.3 (c, 1.1 in  $CHCl_3$ )

References: