



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

**Molecular Formula:** C<sub>27</sub>H<sub>46</sub>O<sub>2</sub>

**Molecular Weight:** 402.659

**Accurate Mass:** 402.34978

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

>>Variant: 3 $\alpha$ -form

**Molecular Formula:** C<sub>27</sub>H<sub>46</sub>O<sub>2</sub>

**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:** [ $\alpha$ ]<sub>D</sub><sup>28</sup> -41.5 (CHCl<sub>3</sub>)

>>Derivative: 3-Ac

**CAS Registry Number:** 67371-50-0

**Molecular Formula:** C<sub>29</sub>H<sub>48</sub>O<sub>3</sub>

**Molecular Weight:** 444.696

**Accurate Mass:** 444.360345

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

**Physical Description:** Oil

>>Variant: 3 $\beta$ -form

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

**CAS Registry Number:** 2140-46-7

**Molecular Formula:** C<sub>27</sub>H<sub>46</sub>O<sub>2</sub>

**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:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> -39 (c, 1.05 in CHCl<sub>3</sub>)

**Fluka:** 55125

**Sigma:** H1015

>>Derivative: 3-Ac

**CAS Registry Number:** 10525-22-1

**Molecular Formula:** C<sub>29</sub>H<sub>48</sub>O<sub>3</sub>

**Molecular Weight:** 444.696

**Accurate Mass:** 444.360345

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

**Physical Description:** Cryst. (Me<sub>2</sub>CO)

**Melting Point:** Mp 139-140°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> -41.4 (c, 1.05 in CHCl<sub>3</sub>)

>>Derivative: Di-Ac

**CAS Registry Number:** 59975-17-6

**Molecular Formula:** C<sub>31</sub>H<sub>50</sub>O<sub>4</sub>

**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°