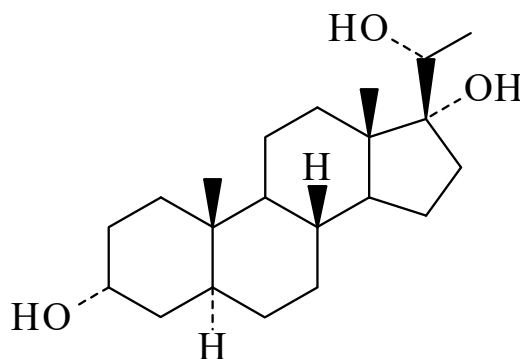




>>Entry Name: Pregnane-3,17,20-triol, 9CI



Extra CAS Registry Numbers(s): 27178-64-9

**Molecular Formula:** C<sub>21</sub>H<sub>36</sub>O<sub>3</sub>

**Molecular Weight:** 336.514

**Accurate Mass:** 336.266445

**Percentage Composition:** C 74.95%; H 10.78%; O 14.26%

>>Variant: (3 $\alpha$ ,5 $\alpha$ ,17 $\alpha$ OH,20*R*)-form

Synonym(s): (3 $\alpha$ ,5 $\alpha$ ,17 $\alpha$ OH,20 $\beta$ )-form

**CAS Registry Number:** 13933-75-0

**Molecular Formula:** C<sub>21</sub>H<sub>36</sub>O<sub>3</sub>

**Molecular Weight:** 336.514

**Accurate Mass:** 336.266445

**Percentage Composition:** C 74.95%; H 10.78%; O 14.26%

**Physical Description:** Cryst. (EtOAc)

**Melting Point:** Mp 226-229°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>25</sup> -5.8 (CHCl<sub>3</sub>)

**Sigma:** P2507

>>Variant: (3 $\alpha$ ,5 $\alpha$ ,17 $\alpha$ OH,20*S*)-form

Synonym(s): (3 $\alpha$ ,5 $\alpha$ ,17 $\alpha$ OH,20 $\alpha$ )-form

**CAS Registry Number:** 16134-59-1

**Molecular Formula:** C<sub>21</sub>H<sub>36</sub>O<sub>3</sub>

**Molecular Weight:** 336.514

**Accurate Mass:** 336.266445

**Percentage Composition:** C 74.95%; H 10.78%; O 14.26%

**Melting Point:** Mp 228-230°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>26</sup> -13.2 (CHCl<sub>3</sub>)

>>Derivative: 20-Ac

**Molecular Formula:** C<sub>23</sub>H<sub>38</sub>O<sub>4</sub>

**Molecular Weight:** 378.551

**Accurate Mass:** 378.27701

**Percentage Composition:** C 72.98%; H 10.12%; O 16.91%

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

**Melting Point:** Mp 213-216.5°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>28</sup> -20.7 (CHCl<sub>3</sub>)

>>Derivative: 3,20-Di-Ac

**Molecular Formula:** C<sub>25</sub>H<sub>40</sub>O<sub>5</sub>

**Molecular Weight:** 420.588

**Accurate Mass:** 420.287575

**Percentage Composition:** C 71.39%; H 9.59%; O 19.02%

**Melting Point:** Mp 123-124 and 130-131° (double Mp)

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>22</sup> -15.7 (CHCl<sub>3</sub>)