



**CAS Registry Number:** 95826-69-0  
**Molecular Formula:** C<sub>25</sub>H<sub>38</sub>O<sub>7</sub>  
**Molecular Weight:** 450.571  
**Accurate Mass:** 450.261755  
**Percentage Composition:** C 66.64%; H 8.50%; O 24.86%  
**Physical Description:** Leaflets (Me<sub>2</sub>CO/Et<sub>2</sub>O)  
**Melting Point:** Mp 182-183°  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>22</sup>+69 (c, 1.5 in CHCl<sub>3</sub>)

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

Synonym(s):  $\alpha$ -Cortolone

**CAS Registry Number:** 516-42-7

**Molecular Formula:** C<sub>21</sub>H<sub>34</sub>O<sub>5</sub>  
**Molecular Weight:** 366.497  
**Accurate Mass:** 366.240625  
**Percentage Composition:** C 68.82%; H 9.35%; O 21.83%  
**Biological Source:** Constit. of human urine  
**Physical Description:** Cryst. (MeOH/EtOAc)  
**Melting Point:** Mp 208-210°  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub> +44 (EtOH)  
**Sigma:** C5381

>>Derivative: 20,21-Di-Ac

**CAS Registry Number:** 95826-64-5  
**Physical Description:** Needles (Me<sub>2</sub>CO aq.)  
**Melting Point:** Mp 200-201°  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>23</sup>+6 (c, 0.56 in CHCl<sub>3</sub>)

>>Derivative: 3,20,21-Tri-Ac

**Melting Point:** Mp 216-217°  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>24</sup>+28.5 (c, 0.5 in dioxan)

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

**Molecular Formula:** C<sub>21</sub>H<sub>34</sub>O<sub>5</sub>  
**Molecular Weight:** 366.497  
**Accurate Mass:** 366.240625  
**Percentage Composition:** C 68.82%; H 9.35%; O 21.83%  
**Melting Point:** Mp 177-180°

>>Derivative: 3,20,21-Tri-Ac

**Melting Point:** Mp 205-206°

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

**Molecular Formula:** C<sub>21</sub>H<sub>34</sub>O<sub>5</sub>  
**Molecular Weight:** 366.497  
**Accurate Mass:** 366.240625  
**Percentage Composition:** C 68.82%; H 9.35%; O 21.83%

>>Derivative: 20,21-Di-Ac

**Physical Description:** Cryst. (CHCl<sub>3</sub>/MeOH)  
**Melting Point:** Mp 280-282°  
**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>26</sup>+5.2 (CHCl<sub>3</sub>)

References: