



**Melting Point:** Mp 257-260° (as Na salt)

>>**Derivative:** 3-Sulfate

**Melting Point:** Mp 232-234 as° (K salt)

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

**CAS Registry Number:** 516-55-2

**Molecular Formula:** C<sub>21</sub>H<sub>34</sub>O<sub>2</sub>

**Molecular Weight:** 318.498

**Accurate Mass:** 318.25588

**Percentage Composition:** C 79.19%; H 10.76%; O 10.05%

**Physical Description:** Cryst. (Me<sub>2</sub>CO/hexane) or needles (C<sub>6</sub>H<sub>6</sub>)

**Melting Point:** Mp 194.5°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub><sup>30</sup>+87 (c, 1 in CHCl<sub>3</sub>)

**Rare Chemicals Library:** S36271-9

**Sigma:** P7879

>>**Derivative:** Oxime

**Molecular Formula:** C<sub>21</sub>H<sub>35</sub>NO<sub>2</sub>

**Molecular Weight:** 333.513

**Accurate Mass:** 333.266779

**Percentage Composition:** C 75.63%; H 10.58%; N 4.20%; O 9.59%

**Physical Description:** Cryst. (EtOH aq.)

**Melting Point:** Mp 231-232°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub> +30 (c, 2.3 in Py)

>>**Derivative:** Ac

**CAS Registry Number:** 906-83-2

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

**Melting Point:** Mp 157-159° (149°)

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub> +73 (c, 0.3 in CHCl<sub>3</sub>). [ $\alpha$ ]<sub>D</sub><sup>20</sup>+23.5 (c, 2 in CHCl<sub>3</sub>)

**Rare Chemicals Library:** S39652-4

**Sigma:** P8004

>>**Derivative:** 3-Sulfate

**Melting Point:** Mp 207-208° (as K salt)

>>**Derivative:** 3-Me ether

**Synonym(s):** 3 $\beta$ -Methoxy-5 $\alpha$ -pregnan-20-one

**CAS Registry Number:** 7680-01-5

**Molecular Formula:** C<sub>22</sub>H<sub>36</sub>O<sub>2</sub>

**Molecular Weight:** 332.525

**Accurate Mass:** 332.27153

**Percentage Composition:** C 79.47%; H 10.91%; O 9.62%

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

**Melting Point:** Mp 123-124°

**Optical Rotation:** [ $\alpha$ ]<sub>D</sub> +89 (c, 3.4 in CHCl<sub>3</sub>)

>>**Derivative:** 3-O- $\beta$ -D-Glucopyranosiduronic acid

**Molecular Formula:** C<sub>27</sub>H<sub>42</sub>O<sub>8</sub>

**Molecular Weight:** 494.624

**Accurate Mass:** 494.28797

**Percentage Composition:** C 65.56%; H 8.56%; O 25.88%

**Melting Point:** Mp 202-202° (as 2',3',4'-Tri-Ac, Me ester)