

# 5-Pregnene-3«beta»,20«alpha»,21-triol

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C21H34O3/c1-20-9-7-14(23)11-13(20)3-4-15-16-5-6-18(19(24)12-22)21(16,2)1 |
| <b>InchiKey:</b>            | DAXILKUPMDAOAK-AKTIQGTHSA-N   |
| <b>Formula:</b>             | C21H34O3  |
| <b>SMILES:</b>              | CC12CCC(O)CC1=CCC1C2CCC2(C)C(C(O)CO)CCC12   |
| <b>Mol. weight [g/mol]:</b> | 334.49  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -118.24 | kJ/mol               | Joback Method  |
| hf            | -662.57 | kJ/mol               | Joback Method  |
| hfus          | 32.38   | kJ/mol               | Joback Method  |
| hvap          | 110.23  | kJ/mol               | Joback Method  |
| log10ws       | -4.61   |                      | Crippen Method |
| logp          | 3.280   |                      | Crippen Method |
| mvol          | 276.620 | ml/mol               | McGowan Method |
| pc            | 1901.92 | kPa                  | Joback Method  |
| rmpol         | 2960.00 |                      | NIST Webbook   |
| rmpol         | 2960.00 |                      | NIST Webbook   |
| tb            | 994.90  | K                    | Joback Method  |
| tc            | 1218.95 | K                    | Joback Method  |
| tf            | 596.41  | K                    | Joback Method  |
| vc            | 1.030   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1083.83 | J/molxK | 994.90          | Joback Method |
| cpg           | 1110.61 | J/molxK | 1032.24         | Joback Method |
| cpg           | 1138.60 | J/molxK | 1069.58         | Joback Method |
| cpg           | 1168.12 | J/molxK | 1106.93         | Joback Method |
| cpg           | 1199.47 | J/molxK | 1144.27         | Joback Method |
| cpg           | 1232.98 | J/molxK | 1181.61         | Joback Method |
| cpg           | 1268.96 | J/molxK | 1218.95         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R528846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R528846&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

# Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>h vap:</b>   | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>m cvol:</b>  | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>r inpol:</b> | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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