

# Androsten-17-(beta)-ol-3-one, 17(alpha)-methyl-delta<sup>4</sup>-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Androsten-17-(beta)-ol-3-one, 17(alpha)-methyl-delta                               |
| <b>Inchi:</b>               | InChI=1S/C20H30O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1) |
| <b>InchiKey:</b>            | GCKMFJBGXUYNAG-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C20H30O2   |
| <b>SMILES:</b>              | CC12CCC(=O)C=C1CCC1C2CCC2(C)C1CCC2(C)O   |
| <b>Mol. weight [g/mol]:</b> | 302.45   |
| <b>CAS:</b>                 | 2607-14-9  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 29.05   | kJ/mol               | Joback Method  |
| hf            | -434.31 | kJ/mol               | Joback Method  |
| hfus          | 17.28   | kJ/mol               | Joback Method  |
| hvap          | 78.43   | kJ/mol               | Joback Method  |
| log10ws       | -5.07   |                      | Crippen Method |
| logp          | 4.269   |                      | Crippen Method |
| mcvol         | 252.360 | ml/mol               | McGowan Method |
| pc            | 1930.44 | kPa                  | Joback Method  |
| tb            | 860.83  | K                    | Joback Method  |
| tc            | 1100.51 | K                    | Joback Method  |
| tf            | 574.86  | K                    | Joback Method  |
| vc            | 0.948   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 898.24  | J/molxK | 860.83          | Joback Method |
| cpg           | 925.32  | J/molxK | 900.78          | Joback Method |
| cpg           | 953.37  | J/molxK | 940.72          | Joback Method |
| cpg           | 982.85  | J/molxK | 980.67          | Joback Method |
| cpg           | 1014.21 | J/molxK | 1020.62         | Joback Method |
| cpg           | 1047.90 | J/molxK | 1060.56         | Joback Method |
| cpg           | 1084.38 | J/molxK | 1100.51         | 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=C2607149&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2607149&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvap:</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>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <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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