# Androstane-3,17-diol, 17-methyl-, (3«alpha»,5«alpha»,17«beta»)-

**Other names:** Ba 2664
5«alpha»-Androstane-3«alpha»,17«beta»-diol, 17-methyl-
17«alpha»-Methyl-5«alpha»-androstane-3«alpha»,17«beta»-diol
17«alpha»-Methyl-5«alpha»-androstan-3«alpha»,17«beta»-diol
17-«beta»-Methyl-5-«alpha»-androstan-3-«alpha»,17-«alpha»-diol
5alpha-Androstan-3alpha,17beta-diol, 17alpha-methyl
5A-Androstan-3A,17B-diol, 17A-methyl

**Inchi:** InChI=1S/C20H34O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1

**InchiKey:** QGKQXZFZOIQFBI-RZEMGSGWSA-N

**Formula:** C20H34O2

**SMILES:** CC12CCC(O)CC1CCC1C2CCC2(C)C1CCC2(C)O

**Mol. weight [g/mol]:** 306.48

**CAS:** 641-82-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -20.93 | kJ/mol | Joback Method |
| hf | -535.83 | kJ/mol | Joback Method |
| hfus | 23.16 | kJ/mol | Joback Method |
| hvap | 89.30 | kJ/mol | Joback Method |
| log10ws | -5.07 | | Crippen Method |
| logp | 4.141 | | Crippen Method |
| mcvol | 260.960 | ml/mol | McGowan Method |
| pc | 1880.53 | kPa | Joback Method |
| rinpol | 2568.00 | | NIST Webbook |
| rinpol | 2568.00 | | NIST Webbook |
| rinpol | 2564.00 | | NIST Webbook |
| tb | 871.71 | K | Joback Method |
| tc | 1089.20 | K | Joback Method |
| tf | 545.70 | K | Joback Method |
| vc | 0.972 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 967.80 | J/mol×K | 871.71 | Joback Method |
| cpg | 993.94 | J/mol×K | 907.96 | Joback Method |
| cpg | 1020.92 | J/mol×K | 944.21 | Joback Method |
| cpg | 1049.12 | J/mol×K | 980.46 | Joback Method |
| cpg | 1078.90 | J/mol×K | 1016.70 | Joback Method |
| cpg | 1110.63 | J/mol×K | 1052.95 | Joback Method |
| cpg | 1144.66 | J/mol×K | 1089.20 | Joback Method |

# Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C641827&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

# Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.