# Cycloandrostan-6,17-dione, 3alpha,5alpha-

**Inchi:** InChI=1S/C19H26O2/c1-17-7-6-14-12(13(17)3-4-15(17)20)9-16(21)19-10-11(19)5-8-18(1
**InchiKey:** ABXKYAJHLPGJLD-UHFFFAOYSA-N
**Formula:** C19H26O2
**SMILES:** CC12CCC3C(CC(=O)C45CC4CCC35C)C1CCC2=O
**Mol. weight [g/mol]:** 286.41
**CAS:** 13713-90-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 111.58 | kJ/mol | Joback Method |
| hf | -354.17 | kJ/mol | Joback Method |
| hfus | 13.71 | kJ/mol | Joback Method |
| hvap | 62.22 | kJ/mol | Joback Method |
| log10ws | -4.12 | | Crippen Method |
| logp | 3.777 | | Crippen Method |
| mcvol | 227.410 | ml/mol | McGowan Method |
| pc | 2060.49 | kPa | Joback Method |
| tb | 803.38 | K | Joback Method |
| tc | 1069.44 | K | Joback Method |
| tf | 586.21 | K | Joback Method |
| vc | 0.875 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 801.12 | J/mol×K | 803.38 | Joback Method |
| cpg | 829.16 | J/mol×K | 847.72 | Joback Method |
| cpg | 857.96 | J/mol×K | 892.07 | Joback Method |
| cpg | 888.20 | J/mol×K | 936.41 | Joback Method |
| cpg | 920.52 | J/mol×K | 980.75 | Joback Method |
| cpg | 955.60 | J/mol×K | 1025.09 | Joback Method |
| cpg | 994.08 | J/mol×K | 1069.44 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C13713901&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

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|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |