# 5-«beta»-Androstan-3-«beta»,17-«beta»-diol, TFA

**Inchi:** InChI=1S/C23H30F6O4/c1-20-9-7-13(32-18(30)22(24,25)26)11-12(20)3-4-14-15-5-6-17(

**InchiKey:** NXQFDYRIAIABNB-MWBOZAONSA-N

**Formula:** C23H30F6O4

**SMILES:** CC12CCC(OC(=O)C(F)(F)F)CC1CCC1C2CCC2(C)C(OC(=O)C(F)(F)F)CCC12

**Mol. weight [g/mol]:** 484.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1347.56 | kJ/mol | Joback Method |
| hf | -1992.29 | kJ/mol | Joback Method |
| hfus | 38.28 | kJ/mol | Joback Method |
| hvap | 74.58 | kJ/mol | Joback Method |
| log10ws | -6.85 | | Crippen Method |
| logp | 5.977 | | Crippen Method |
| mcvol | 316.990 | ml/mol | McGowan Method |
| pc | 1139.03 | kPa | Joback Method |
| rinpol | 2279.00 | | NIST Webbook |
| rinpol | 2295.00 | | NIST Webbook |
| tb | 897.49 | K | Joback Method |
| tc | 1110.56 | K | Joback Method |
| tf | 586.67 | K | Joback Method |
| vc | 1.238 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1166.32 | J/mol×K | 897.49 | Joback Method |
| cpg | 1190.15 | J/mol×K | 933.00 | Joback Method |
| cpg | 1214.03 | J/mol×K | 968.51 | Joback Method |
| cpg | 1238.23 | J/mol×K | 1004.03 | Joback Method |
| cpg | 1263.04 | J/mol×K | 1039.54 | Joback Method |
| cpg | 1288.73 | J/mol×K | 1075.05 | Joback Method |
| cpg | 1315.58 | J/mol×K | 1110.56 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R385129&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |