6Beta-fluoro-17beta-hydroxyandrost-4-en-3-one

Inchi: InChI=1S/C19H27FO2/c1-18-7-5-11(21)9-15(18)16(20)10-12-13-3-4-17(22)19(13,2)8-6-1
InchiKey: GGQPTOITOZXLBE-UHFFFAOYSA-N
Formula: C19H27FO2
SMILES: CC12CCC(=O)C=C1C(F)CC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]: 306.41
CAS: 1852-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-176.40	kJ/mol	Joback Method
hf	-645.36	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	76.23	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.827		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
tb	832.31	K	Joback Method
tc	1060.49	K	Joback Method
tf	536.04	K	Joback Method
vc	0.910	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	849.85	J/mol×K	832.31	Joback Method
cpg	872.98	J/mol×K	870.34	Joback Method
cpg	895.99	J/mol×K	908.37	Joback Method
cpg	919.14	J/mol×K	946.40	Joback Method
cpg	942.72	J/mol×K	984.43	Joback Method
cpg	967.02	J/mol×K	1022.46	Joback Method
cpg	992.31	J/mol×K	1060.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1852580&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume