4-Fluoro-17beta-hydroxyandrost-4-en-3-one

Inchi: InChI=1S/C19H27FO2/c1-18-10-8-15(21)17(20)14(18)4-3-11-12-5-6-16(22)19(12,2)9-7-1
InchiKey: MXMZKEJZVAOVLU-UHFFFAOYSA-N
Formula: C19H27FO2
SMILES: CC12CCC(=O)C(F)=C1CCC1C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]: 306.41
CAS: 1649-25-8

Physical Properties

Property code	Value	Unit	Source
gf	-178.32	kJ/mol	Joback Method
hf	-636.49	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	77.21	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	4.176		Crippen Method
mcvol	240.040	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
tb	841.96	K	Joback Method
tc	1070.90	K	Joback Method
tf	552.80	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	846.54	J/mol×K	841.96	Joback Method
cpg	869.48	J/mol×K	880.12	Joback Method
cpg	892.42	J/mol×K	918.27	Joback Method
cpg	915.64	J/mol×K	956.43	Joback Method
cpg	939.43	J/mol×K	994.59	Joback Method
cpg	964.08	J/mol×K	1032.74	Joback Method
cpg	989.87	J/mol×K	1070.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1649258&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