5A-Estran-3A,17B-diol, 17A-methyl

Inchi: InChI=1S/C19H32O2/c1-18-9-7-15-14-6-4-13(20)11-12(14)3-5-16(15)17(18)8-10-19(18,2
InchiKey: HMMIGANEGZIQOT-KIYNURMZSA-N
Formula: C19H32O2
SMILES: CC1(O)CCC2C3CCC4CC(O)CCC4C3CCC21C
Mol. weight [g/mol]: 292.46

Physical Properties

Property code	Value	Unit	Source
gf	-23.86	kJ/mol	Joback Method
hf	-530.43	kJ/mol	Joback Method
hfus	26.87	kJ/mol	Joback Method
hvap	88.22	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.751		Crippen Method
mcvol	246.870	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	2395.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	848.59	K	Joback Method
tc	1062.44	K	Joback Method
tf	510.53	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	907.30	J/mol×K	848.59	Joback Method
cpg	930.23	J/mol×K	884.23	Joback Method
cpg	953.16	J/mol×K	919.87	Joback Method
cpg	976.35	J/mol×K	955.52	Joback Method
cpg	1000.05	J/mol×K	991.16	Joback Method
cpg	1024.53	J/mol×K	1026.80	Joback Method
cpg	1050.06	J/mol×K	1062.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R5506&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