3«beta»,16a-dihydroxy-5-androstene-17-one

Inchi: InChI=1S/C17H24O3/c18-10-2-4-11-9(7-10)1-3-13-12(11)5-6-14-15(13)8-16(19)17(14)20
InchiKey: YMRBSMNGYQGMRQ-SYCCPWCRSA-N
Formula: C17H24O3
SMILES: O=C1C(O)CC2C1CCC1C3CCC(O)CC3=CCC21
Mol. weight [g/mol]: 276.37

Physical Properties

Property code	Value	Unit	Source
gf	-124.27	kJ/mol	Joback Method
hf	-590.68	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	91.58	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.070		Crippen Method
mcvol	215.960	ml/mol	McGowan Method
pc	2347.36	kPa	Joback Method
rinpol	2774.00		NIST Webbook
rinpol	2774.00		NIST Webbook
tb	878.98	K	Joback Method
tc	1098.15	K	Joback Method
tf	525.93	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.70	J/mol×K	878.98	Joback Method
cpg	813.07	J/mol×K	915.51	Joback Method
cpg	828.21	J/mol×K	952.04	Joback Method
cpg	842.18	J/mol×K	988.56	Joback Method
cpg	855.07	J/mol×K	1025.09	Joback Method
cpg	866.93	J/mol×K	1061.62	Joback Method
cpg	877.85	J/mol×K	1098.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R249008&Units=SI

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