3«alpha»-hydroxy-5«beta»-androstane-17-one

Inchi: InChI=1S/C17H26O2/c18-11-2-4-12-10(9-11)1-3-14-13(12)5-6-16-15(14)7-8-17(16)19/h1
InchiKey: VAAOCLICQGAZPU-LRGVGNOESA-N
Formula: C17H26O2
SMILES: O=C1CCC2C1CCC1C3CCC(O)CC3CCC21
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	-7.78	kJ/mol	Joback Method
hf	-484.76	kJ/mol	Joback Method
hfus	28.64	kJ/mol	Joback Method
hvap	73.95	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.179		Crippen Method
mcvol	214.390	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	2547.00		NIST Webbook
tb	782.66	K	Joback Method
tc	1009.96	K	Joback Method
tf	451.83	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	758.53	J/mol×K	782.66	Joback Method
cpg	780.07	J/mol×K	820.54	Joback Method
cpg	800.04	J/mol×K	858.43	Joback Method
cpg	818.50	J/mol×K	896.31	Joback Method
cpg	835.54	J/mol×K	934.19	Joback Method
cpg	851.24	J/mol×K	972.07	Joback Method
cpg	865.68	J/mol×K	1009.96	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=R248996&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