11«beta»-hydroxy-etiocholanolone, 3«alpha»,11«beta»-dihydroxy-5«beta»-androstane

Inchi: InChI=1S/C17H26O3/c18-10-2-4-11-9(7-10)1-3-13-12-5-6-15(19)14(12)8-16(20)17(11)13

InchiKey: DQGUTLNRNVUFAI-STEAYNICSA-N

Formula: C17H26O3

SMILES: O=C1CCC2C1CC(O)C1C3CCC(O)CC3CCC21

Mol. weight [g/mol]: 278.39

Physical Properties

Property code	Value	Unit	Source
gf	-152.31	kJ/mol	Joback Method
hf	-657.33	kJ/mol	Joback Method
hfus	33.80	kJ/mol	Joback Method
hvap	90.32	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.150		Crippen Method
mcvol	220.260	ml/mol	McGowan Method
pc	2229.20	kPa	Joback Method
rinpol	2731.00		NIST Webbook
tb	870.17	K	Joback Method
tc	1087.24	K	Joback Method
tf	508.41	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.48	J/mol×K	870.17	Joback Method
cpg	848.01	J/mol×K	906.35	Joback Method
cpg	864.20	J/mol×K	942.53	Joback Method
cpg	879.12	J/mol×K	978.71	Joback Method
cpg	892.83	J/mol×K	1014.89	Joback Method
cpg	905.39	J/mol×K	1051.06	Joback Method
cpg	916.88	J/mol×K	1087.24	Joback Method

Sources

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=R248867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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