11-keto-etiocholanolone, 3«alpha»-hydroxy-5«beta»-androstane-11,17-dion

Inchi: InChI=1S/C17H24O3/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: ZCVBLANICGCTOM-IKZQXDISSA-N

Formula: C17H24O3

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

Mol. weight [g/mol]: 276.37

Physical Properties

Property code	Value	Unit	Source
gf	-130.37	kJ/mol	Joback Method
hf	-622.46	kJ/mol	Joback Method
hfus	28.15	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	2.358		Crippen Method
mcvol	215.960	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	2634.00		NIST Webbook
tb	850.48	K	Joback Method
tc	1087.38	K	Joback Method
tf	520.05	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.25	J/mol×K	850.48	Joback Method
cpg	815.76	J/mol×K	889.96	Joback Method
cpg	833.54	J/mol×K	929.45	Joback Method
cpg	849.62	J/mol×K	968.93	Joback Method
cpg	864.08	J/mol×K	1008.41	Joback Method
cpg	876.94	J/mol×K	1047.90	Joback Method
cpg	888.27	J/mol×K	1087.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R248872&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