17-epi-Mestanolone

Inchi: InChI=1S/C20H32O2/c1-18-9-6-14(21)12-13(18)4-5-15-16(18)7-10-19(2)17(15)8-11-20(1
InchiKey: WYZDXEKUWRCKOB-QLCSRNHCSA-N
Formula: C20H32O2
SMILES: CC12CCC(=O)CC1CCC1C2CCC2(C)C1CCC2(C)O
Mol. weight [g/mol]: 304.47

Physical Properties

Property code	Value	Unit	Source
gf	1.01	kJ/mol	Joback Method
hf	-500.96	kJ/mol	Joback Method
hfus	17.51	kJ/mol	Joback Method
hvap	77.17	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.349		Crippen Method
mcvol	256.660	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	2605.00		NIST Webbook
rinpol	2605.00		NIST Webbook
tb	852.02	K	Joback Method
tc	1089.40	K	Joback Method
tf	557.34	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.72	J/mol×K	852.02	Joback Method
cpg	957.55	J/mol×K	891.58	Joback Method
cpg	986.09	J/mol×K	931.15	Joback Method
cpg	1015.78	J/mol×K	970.71	Joback Method
cpg	1047.06	J/mol×K	1010.27	Joback Method
cpg	1080.37	J/mol×K	1049.84	Joback Method
cpg	1116.14	J/mol×K	1089.40	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=R257777&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