8-Dehydro DHEA

Inchi: InChI=1S/C19H30O2/c1-18-9-7-13(20)11-12(18)3-4-14-15-5-6-17(21)19(15,2)10-8-16(14
InchiKey: MHRBIDJSVFENIX-TWYPGWQISA-N
Formula: C19H30O2
SMILES: CC12CCC(O)CC1CCC1=C2CCC2(C)C(O)CCC12
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	2.26	kJ/mol	Joback Method
hf	-454.91	kJ/mol	Joback Method
hfus	25.17	kJ/mol	Joback Method
hvap	90.45	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.815		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2608.00		NIST Webbook
rinpol	2608.00		NIST Webbook
tb	867.05	K	Joback Method
tc	1084.05	K	Joback Method
tf	544.81	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.02	J/mol×K	867.05	Joback Method
cpg	894.06	J/mol×K	903.22	Joback Method
cpg	916.42	J/mol×K	939.38	Joback Method
cpg	939.36	J/mol×K	975.55	Joback Method
cpg	963.16	J/mol×K	1011.71	Joback Method
cpg	988.10	J/mol×K	1047.88	Joback Method
cpg	1014.46	J/mol×K	1084.05	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=R304086&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