7-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: UIPWMMPORBHETL-OAQGJJPVSA-N
Formula: C19H30O2
SMILES: CC12CCC3C(=CCC4CC(O)CCC43C)C1CCC2O
Mol. weight [g/mol]: 290.44

Physical Properties

Property code	Value	Unit	Source
gf	4.18	kJ/mol	Joback Method
hf	-463.78	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	89.48	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.671		Crippen Method
mcvol	242.570	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	2630.00		NIST Webbook
tb	857.40	K	Joback Method
tc	1073.36	K	Joback Method
tf	528.05	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	875.45	J/mol×K	857.40	Joback Method
cpg	897.54	J/mol×K	893.39	Joback Method
cpg	919.80	J/mol×K	929.39	Joback Method
cpg	942.52	J/mol×K	965.38	Joback Method
cpg	965.95	J/mol×K	1001.38	Joback Method
cpg	990.39	J/mol×K	1037.37	Joback Method
cpg	1016.09	J/mol×K	1073.36	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=R304071&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