5«beta»-Pregn-7-ene-3«alpha»,20«alpha»-diol

Inchi: InChI=1S/C21H34O2/c1-13(22)17-6-7-18-16-5-4-14-12-15(23)8-10-20(14,2)19(16)9-11-2
InchiKey: OSMCDXKOUCZPDS-GFMBRAFVSA-N
Formula: C21H34O2
SMILES: CC(O)C1CCC2C3=CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	18.58	kJ/mol	Joback Method
hf	-510.34	kJ/mol	Joback Method
hfus	28.29	kJ/mol	Joback Method
hvap	93.55	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.307		Crippen Method
mcvol	270.750	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	2781.00		NIST Webbook
rinpol	2781.00		NIST Webbook
tb	902.72	K	Joback Method
tc	1119.93	K	Joback Method
tf	535.59	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.51	J/mol×K	902.72	Joback Method
cpg	1026.76	J/mol×K	938.92	Joback Method
cpg	1051.43	J/mol×K	975.12	Joback Method
cpg	1076.78	J/mol×K	1011.32	Joback Method
cpg	1103.11	J/mol×K	1047.52	Joback Method
cpg	1130.70	J/mol×K	1083.73	Joback Method
cpg	1159.83	J/mol×K	1119.93	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304031&Units=SI

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