5«beta»-Pregn-8-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: CVXRELSVEQTOQH-VDDUQTHDSA-N
Formula: C21H34O2
SMILES: CC(O)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1CC3
Mol. weight [g/mol]: 318.49

Physical Properties

Property code	Value	Unit	Source
gf	16.66	kJ/mol	Joback Method
hf	-501.47	kJ/mol	Joback Method
hfus	26.83	kJ/mol	Joback Method
hvap	94.52	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	4.451		Crippen Method
mcvol	270.750	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	2741.00		NIST Webbook
rinpol	2741.00		NIST Webbook
tb	912.37	K	Joback Method
tc	1130.79	K	Joback Method
tf	552.35	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.40	J/mol×K	912.37	Joback Method
cpg	1023.77	J/mol×K	948.77	Joback Method
cpg	1048.69	J/mol×K	985.18	Joback Method
cpg	1074.44	J/mol×K	1021.58	Joback Method
cpg	1101.32	J/mol×K	1057.98	Joback Method
cpg	1129.61	J/mol×K	1094.38	Joback Method
cpg	1159.60	J/mol×K	1130.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304051&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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