5,8-Pregnadiene-3«beta»,20«alpha»-diol

Inchi: InChI=1S/C21H32O2/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: NESPUYJOJJTBCC-QGVZDEAMSA-N
Formula: C21H32O2
SMILES: CC(O)C1CCC2C3=C(CCC21C)C1(C)CCC(O)CC1=CC3
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	44.70	kJ/mol	Joback Method
hf	-434.82	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	95.78	kJ/mol	Joback Method
log10ws	-5.68		Crippen Method
logp	4.371		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	2848.00		NIST Webbook
tb	921.18	K	Joback Method
tc	1141.62	K	Joback Method
tf	569.87	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.95	J/mol×K	921.18	Joback Method
cpg	989.80	J/mol×K	957.92	Joback Method
cpg	1014.40	J/mol×K	994.66	Joback Method
cpg	1040.06	J/mol×K	1031.40	Joback Method
cpg	1067.07	J/mol×K	1068.14	Joback Method
cpg	1095.73	J/mol×K	1104.88	Joback Method
cpg	1126.35	J/mol×K	1141.62	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=R304011&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