5,7-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: DOMUDBZFBQTRCJ-AQADCPELSA-N
Formula: C21H32O2
SMILES: CC(O)C1CCC2C3=CC=C4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	46.62	kJ/mol	Joback Method
hf	-443.69	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	94.81	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.227		Crippen Method
mcvol	266.450	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2876.00		NIST Webbook
tb	911.53	K	Joback Method
tc	1130.77	K	Joback Method
tf	553.11	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.32	J/mol×K	911.53	Joback Method
cpg	993.00	J/mol×K	948.07	Joback Method
cpg	1017.28	J/mol×K	984.61	Joback Method
cpg	1042.47	J/mol×K	1021.15	Joback Method
cpg	1068.85	J/mol×K	1057.69	Joback Method
cpg	1096.72	J/mol×K	1094.23	Joback Method
cpg	1126.38	J/mol×K	1130.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R304006&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

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