

5-«alpha»-Pregnane-17-«alpha»,20-«beta»-diol

Inchi:	InChI=1S/C21H36O2/c1-14(22)21(23)13-10-18-16-8-7-15-6-4-5-11-19(15,2)17(16)9-12-2
InchiKey:	BSQKCQWUHC AKQY-BNWHZUCPSA-N
Formula:	C21H36O2
SMILES:	CC(O)C1(O)CCC2C3CCC4CCCCC4(C)C3CCC21C
Mol. weight [g/mol]:	320.51

Physical Properties

Property code	Value	Unit	Source
gf	-7.24	kJ/mol	Joback Method
hf	-541.41	kJ/mol	Joback Method
hfus	21.16	kJ/mol	Joback Method
hvap	91.44	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.531		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	2585.00		NIST Webbook
rinpol	2585.00		NIST Webbook
tb	898.82	K	Joback Method
tc	1118.26	K	Joback Method
tf	546.21	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1030.73	J/mol×K	898.82	Joback Method
cpg	1058.44	J/mol×K	935.39	Joback Method
cpg	1087.30	J/mol×K	971.97	Joback Method
cpg	1117.68	J/mol×K	1008.54	Joback Method
cpg	1149.98	J/mol×K	1045.12	Joback Method
cpg	1184.58	J/mol×K	1081.69	Joback Method
cpg	1221.87	J/mol×K	1118.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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