Allopregnane-3«alpha»,20«alpha»-diol

Other names: Pregnane-3,20-diol, (3«alpha»,5«alpha»,20S)-
5«alpha»-Pregnane-3«alpha»,20«alpha»-diol
Allopregnanediol
3«alpha»,20«alpha»-Dihydroxy-5«alpha»-pregnane
5«alpha»-Pregnanediol
Pregnane-3,20-diol, (3«alpha»,5«alpha»,20«alpha»)-
Pregnan-3A,20A-diol
5.beta.-Pregnane-3.alpha.,20.alpha.-diol
Pregnane-3,20-diol

Inchi: InChI=1S/C21H36O2/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: YWYQTGBBEZQBGO-UHFFFAOYSA-N

Formula: C21H36O2

SMILES: CC(O)C1CCC2C3CCC4CC(O)CCC4(C)C3CCC12C

Mol. weight [g/mol]: 320.51

CAS: 566-58-5

Physical Properties

Property code	Value	Unit	Source
gf	-9.46	kJ/mol	Joback Method
hf	-576.99	kJ/mol	Joback Method
hfus	28.53	kJ/mol	Joback Method
hvap	92.28	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.387		Crippen Method
mcvol	275.050	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2769.00		NIST Webbook
rinpol	2770.00		NIST Webbook
rinpol	2803.50		NIST Webbook
tb	893.91	K	Joback Method
tc	1109.08	K	Joback Method
tf	518.07	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.23	J/mol×K	893.91	Joback Method
cpg	1060.13	J/mol×K	929.77	Joback Method
cpg	1085.24	J/mol×K	965.63	Joback Method
cpg	1110.84	J/mol×K	1001.50	Joback Method
cpg	1137.20	J/mol×K	1037.36	Joback Method
cpg	1164.59	J/mol×K	1073.22	Joback Method
cpg	1193.29	J/mol×K	1109.08	Joback Method

Sources

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=C566585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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