5-«alpha»-Pregnane-3-«beta»,17-«alpha»,20-«beta

Inchi: InChI=1S/C21H36O3/c1-13(22)21(24)11-8-18-16-5-4-14-12-15(23)6-9-19(14,2)17(16)7-1
InchiKey: SCPADBBISMMJAW-DUBOSXLPSA-N
Formula: C21H36O3
SMILES: CC(O)C1(O)CCC2C3CCC4CC(O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 336.51

Physical Properties

Property code	Value	Unit	Source
gf	-151.77	kJ/mol	Joback Method
hf	-713.98	kJ/mol	Joback Method
hfus	26.32	kJ/mol	Joback Method
hvap	107.81	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	3.502		Crippen Method
mcvol	280.920	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	2845.00		NIST Webbook
tb	986.33	K	Joback Method
tc	1209.67	K	Joback Method
tf	602.79	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.32	J/mol×K	986.33	Joback Method
cpg	1156.05	J/mol×K	1023.55	Joback Method
cpg	1189.85	J/mol×K	1060.78	Joback Method
cpg	1226.10	J/mol×K	1098.00	Joback Method
cpg	1265.22	J/mol×K	1135.22	Joback Method
cpg	1307.60	J/mol×K	1172.45	Joback Method
cpg	1353.64	J/mol×K	1209.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149983&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