3«alpha»,11«beta»,21-trihydroxy-5«alpha»-pregna

Inchi: InChI=1S/C19H30O4/c20-9-18(23)14-6-5-13-15-3-1-10-7-11(21)2-4-12(10)19(15)17(22)8

InchiKey: YIURNAFXNWMMCO-ITRQNZALSA-N

Formula: C19H30O4

SMILES: O=C(CO)C1CCC2C1CC(O)C1C3CCC(O)CC3CCC21

Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-286.33	kJ/mol	Joback Method
hf	-846.06	kJ/mol	Joback Method
hfus	46.22	kJ/mol	Joback Method
hvap	113.64	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.758		Crippen Method
mcvol	254.310	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	3016.00		NIST Webbook
tb	989.49	K	Joback Method
tc	1211.68	K	Joback Method
tf	569.24	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1001.23	J/mol×K	989.49	Joback Method
cpg	1068.47	J/mol×K	1174.65	Joback Method
cpg	1056.80	J/mol×K	1137.62	Joback Method
cpg	1044.35	J/mol×K	1100.59	Joback Method
cpg	1031.01	J/mol×K	1063.55	Joback Method
cpg	1016.67	J/mol×K	1026.52	Joback Method
cpg	1079.45	J/mol×K	1211.68	Joback Method
dvisc	0.0000176	Pa×s	989.49	Joback Method
dvisc	0.0000265	Pa×s	919.45	Joback Method

dvisc	0.0000424	Pa×s	849.41	Joback Method
dvisc	0.0000741	Pa×s	779.37	Joback Method
dvisc	0.0001445	Pa×s	709.32	Joback Method
dvisc	0.0003261	Pa×s	639.28	Joback Method
dvisc	0.0008992	Pa×s	569.24	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=R248901&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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