

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

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:	YIURNAFXNWMCO-VFFFOYLWSA-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	3000.00		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/molxK	989.49	Joback Method
cpg	1016.67	J/molxK	1026.52	Joback Method
cpg	1031.01	J/molxK	1063.55	Joback Method
cpg	1044.35	J/molxK	1100.59	Joback Method
cpg	1056.80	J/molxK	1137.62	Joback Method
cpg	1068.47	J/molxK	1174.65	Joback Method
cpg	1079.45	J/molxK	1211.68	Joback Method
dvisc	0.0008992	Paxs	569.24	Joback Method
dvisc	0.0003261	Paxs	639.28	Joback Method

dvisc	0.0001445	Paxs	709.32	Joback Method
dvisc	0.0000741	Paxs	779.37	Joback Method
dvisc	0.0000424	Paxs	849.41	Joback Method
dvisc	0.0000265	Paxs	919.45	Joback Method
dvisc	0.0000176	Paxs	989.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R248916&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

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