3«alpha»,17«alpha»,21-trihydroxy-5«alpha»-pregn

Inchi: InChI=1S/C19H28O5/c20-9-17(23)19(24)6-5-13-14-3-1-10-7-11(21)2-4-12(10)18(14)16(2
InchiKey: OHOZNBWGXNMTTI-GCSXCLADSA-N
Formula: C19H28O5
SMILES: O=C1CC2C(CCC2(O)C(=O)CO)C2CCC3CC(O)CCC3C12
Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-406.70	kJ/mol	Joback Method
hf	-948.18	kJ/mol	Joback Method
hfus	38.37	kJ/mol	Joback Method
hvap	117.04	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	1.081		Crippen Method
mcvol	255.880	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook
tb	1062.22	K	Joback Method
tc	1300.50	K	Joback Method
tf	665.60	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.83	J/mol×K	1062.22	Joback Method
cpg	1058.28	J/mol×K	1101.93	Joback Method
cpg	1078.85	J/mol×K	1141.65	Joback Method
cpg	1099.75	J/mol×K	1181.36	Joback Method
cpg	1121.17	J/mol×K	1221.07	Joback Method
cpg	1143.34	J/mol×K	1260.79	Joback Method
cpg	1166.47	J/mol×K	1300.50	Joback Method

Sources

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=R248941&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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