3«alpha»,11«beta»,17«alpha»,21-tetrahydroxy-5«a

Inchi: InChI=1S/C19H30O5/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: ZOOTXDVRRFYUOX-YWWCMZMESA-N
Formula: C19H30O5
SMILES: O=C(CO)C1(O)CCC2C3CCC4CC(O)CCC4C3C(O)CC21
Mol. weight [g/mol]: 338.44

Physical Properties

Property code	Value	Unit	Source
gf	-428.64	kJ/mol	Joback Method
hf	-983.05	kJ/mol	Joback Method
hfus	44.01	kJ/mol	Joback Method
hvap	129.17	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	0.873		Crippen Method
mcvol	260.180	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	3040.00		NIST Webbook
tb	1081.91	K	Joback Method
tc	1329.06	K	Joback Method
tf	653.96	K	Joback Method
vc	0.963	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1076.43	J/mol×K	1081.91	Joback Method
cpg	1099.24	J/mol×K	1123.10	Joback Method
cpg	1122.63	J/mol×K	1164.29	Joback Method
cpg	1146.88	J/mol×K	1205.49	Joback Method
cpg	1172.26	J/mol×K	1246.68	Joback Method
cpg	1199.04	J/mol×K	1287.87	Joback Method
cpg	1227.50	J/mol×K	1329.06	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=R248887&Units=SI

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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