Moretenol (21-epi-22[29]hopenol) acetate

Inchi: InChI=1S/C32H52O2/c1-20(2)22-12-16-29(6)23(22)13-18-31(8)25(29)10-11-26-30(7)17-
InchiKey: JRAYHROVVIBKAS-FMSOXZHVSA-N
Formula: C32H52O2
SMILES: C=C(C)C1CCC2(C)C1CCC1(C)C2CCC2C3(C)CCC(OC(C)=O)C(C)(C)C3CCC21C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	221.37	kJ/mol	Joback Method
hf	-551.77	kJ/mol	Joback Method
hfus	31.84	kJ/mol	Joback Method
hvap	88.38	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.596		Crippen Method
mcvol	410.580	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinpol	3432.00		NIST Webbook
tb	1036.91	K	Joback Method
tc	1284.48	K	Joback Method
tf	669.48	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1684.08	J/mol×K	1036.91	Joback Method
cpg	1743.36	J/mol×K	1078.17	Joback Method
cpg	1808.04	J/mol×K	1119.43	Joback Method
cpg	1878.93	J/mol×K	1160.69	Joback Method
cpg	1956.87	J/mol×K	1201.96	Joback Method
cpg	2042.68	J/mol×K	1243.22	Joback Method
cpg	2137.20	J/mol×K	1284.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111354&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