Dammaradienol acetate

Inchi: InChI=1S/C33H54O2/c1-21(2)22(3)11-12-23(4)25-15-19-32(9)26(25)13-14-28-31(8)18-1
InchiKey: BYJGVGIRULHEPW-XKAJVLSQSA-N
Formula: C33H54O2
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CCC2=C(C(C)CC=C(C)C(C)C)CCC23C)C1(C)C
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	207.96	kJ/mol	Joback Method
hf	-577.20	kJ/mol	Joback Method
hfus	36.36	kJ/mol	Joback Method
hvap	94.07	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.296		Crippen Method
mcvol	431.230	ml/mol	McGowan Method
pc	800.24	kPa	Joback Method
rinpol	3334.00		NIST Webbook
tb	1078.27	K	Joback Method
tc	1323.90	K	Joback Method
tf	647.63	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1737.04	J/mol×K	1078.27	Joback Method
cpg	1793.79	J/mol×K	1119.21	Joback Method
cpg	1855.32	J/mol×K	1160.15	Joback Method
cpg	1922.31	J/mol×K	1201.09	Joback Method
cpg	1995.46	J/mol×K	1242.02	Joback Method
cpg	2075.45	J/mol×K	1282.96	Joback Method
cpg	2162.98	J/mol×K	1323.90	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=R111121&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