24-Methylenedammarenol acetate

Inchi: InChI=1S/C33H56O2/c1-21(2)22(3)11-12-23(4)25-15-19-32(9)26(25)13-14-28-31(8)18-1
InchiKey: KESQYNXPZBWPEM-JSRWNDPESA-N
Formula: C33H56O2
SMILES: C=C(CCC(C)C1CCC2(C)C1CCC1C3(C)CCC(OC(C)=O)C(C)(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 484.80

Physical Properties

Property code	Value	Unit	Source
gf	189.46	kJ/mol	Joback Method
hf	-644.51	kJ/mol	Joback Method
hfus	36.58	kJ/mol	Joback Method
hvap	91.20	kJ/mol	Joback Method
log10ws	-9.63		Crippen Method
logp	9.232		Crippen Method
mcvol	435.530	ml/mol	McGowan Method
pc	764.37	kPa	Joback Method
rinpol	3381.00		NIST Webbook
rinpol	3381.00		NIST Webbook
tb	1052.33	K	Joback Method
tc	1292.21	K	Joback Method
tf	616.67	K	Joback Method
vc	1.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1756.23	J/mol×K	1052.33	Joback Method
cpg	1808.78	J/mol×K	1092.31	Joback Method
cpg	1865.11	J/mol×K	1132.29	Joback Method
cpg	1925.84	J/mol×K	1172.27	Joback Method
cpg	1991.60	J/mol×K	1212.25	Joback Method
cpg	2063.01	J/mol×K	1252.23	Joback Method
cpg	2140.70	J/mol×K	1292.21	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=R110539&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