24,24-Dimethyl-9(11)-lanostenol acetate

Inchi: InChI=1S/C34H58O2/c1-22(2)20-30(5,6)21-23(3)25-14-18-34(11)27-12-13-28-31(7,8)29(
InchiKey: KXERJRIPULHEGD-DIQBWDAESA-N
Formula: C34H58O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)CC(C)(C)CC(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 498.82

Physical Properties

Property code	Value	Unit	Source
gf	149.47	kJ/mol	Joback Method
hf	-722.89	kJ/mol	Joback Method
hfus	34.11	kJ/mol	Joback Method
hvap	93.99	kJ/mol	Joback Method
log10ws	-10.04		Crippen Method
logp	9.622		Crippen Method
mcvol	449.620	ml/mol	McGowan Method
pc	735.62	kPa	Joback Method
rinpol	3531.00		NIST Webbook
rinpol	3531.00		NIST Webbook
tb	1084.23	K	Joback Method
tc	1329.65	K	Joback Method
tf	663.60	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1840.30	J/mol×K	1084.23	Joback Method
cpg	1898.20	J/mol×K	1125.13	Joback Method
cpg	1960.81	J/mol×K	1166.04	Joback Method
cpg	2028.83	J/mol×K	1206.94	Joback Method
cpg	2102.97	J/mol×K	1247.85	Joback Method
cpg	2183.92	J/mol×K	1288.75	Joback Method
cpg	2272.39	J/mol×K	1329.65	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=R110148&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