24,25-Dimethyl-9(11)-lanostenol acetate

Inchi: InChI=1S/C34H58O2/c1-21(2)24(5)22(3)20-23(4)26-14-18-34(11)28-12-13-29-31(7,8)30
InchiKey: QQMLGOGDNXLABE-FZYXMIKHSA-N
Formula: C34H58O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)CC(C)C(C)C(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 498.82

Physical Properties

Property code	Value	Unit	Source
gf	141.75	kJ/mol	Joback Method
hf	-724.70	kJ/mol	Joback Method
hfus	34.48	kJ/mol	Joback Method
hvap	94.51	kJ/mol	Joback Method
log10ws	-9.80		Crippen Method
logp	9.478		Crippen Method
mcvol	449.620	ml/mol	McGowan Method
pc	734.42	kPa	Joback Method
rinpol	3501.00		NIST Webbook
tb	1086.58	K	Joback Method
tc	1331.75	K	Joback Method
tf	631.18	K	Joback Method
vc	1.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1842.51	J/mol×K	1086.58	Joback Method
cpg	1899.95	J/mol×K	1127.44	Joback Method
cpg	1961.86	J/mol×K	1168.30	Joback Method
cpg	2028.90	J/mol×K	1209.16	Joback Method
cpg	2101.76	J/mol×K	1250.02	Joback Method
cpg	2181.10	J/mol×K	1290.89	Joback Method
cpg	2267.58	J/mol×K	1331.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110168&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

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