24,25-Dimethyl-9(11),23-lanostadienol acetate

Inchi: InChI=1S/C34H56O2/c1-21(2)24(5)22(3)20-23(4)26-14-18-34(11)28-12-13-29-31(7,8)30
InchiKey: DCHBAAPZUNMZRD-GXKVWZMLSA-N
Formula: C34H56O2
SMILES: CC(=O)OC1CCC2(C)C3=CCC4(C)C(C(C)C=C(C)C(C)C(C)C)CCC4(C)C3CCC2C1(C)C
Mol. weight [g/mol]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	215.86	kJ/mol	Joback Method
hf	-611.99	kJ/mol	Joback Method
hfus	36.89	kJ/mol	Joback Method
hvap	94.93	kJ/mol	Joback Method
log10ws	-9.90		Crippen Method
logp	9.398		Crippen Method
mcvol	445.320	ml/mol	McGowan Method
pc	754.33	kPa	Joback Method
rinpol	3498.00		NIST Webbook
tb	1091.06	K	Joback Method
tc	1338.48	K	Joback Method
tf	627.14	K	Joback Method
vc	1.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1817.56	J/mol×K	1091.06	Joback Method
cpg	1876.58	J/mol×K	1132.30	Joback Method
cpg	1940.53	J/mol×K	1173.53	Joback Method
cpg	2010.12	J/mol×K	1214.77	Joback Method
cpg	2086.04	J/mol×K	1256.01	Joback Method
cpg	2169.03	J/mol×K	1297.24	Joback Method
cpg	2259.77	J/mol×K	1338.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110153&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