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

Inchi: InChI=1S/C34H56O2/c1-22(2)20-30(5,6)21-23(3)25-14-18-34(11)27-12-13-28-31(7,8)29(
InchiKey: SZDMTSJLVIJCPZ-DIQBWDAESA-N
Formula: C34H56O2
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]: 496.81

Physical Properties

Property code	Value	Unit	Source
gf	223.58	kJ/mol	Joback Method
hf	-610.18	kJ/mol	Joback Method
hfus	36.52	kJ/mol	Joback Method
hvap	94.41	kJ/mol	Joback Method
log10ws	-10.14		Crippen Method
logp	9.542		Crippen Method
mcvol	445.320	ml/mol	McGowan Method
pc	755.57	kPa	Joback Method
rinpol	3505.00		NIST Webbook
tb	1088.71	K	Joback Method
tc	1336.64	K	Joback Method
tf	659.56	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1815.36	J/mol×K	1088.71	Joback Method
cpg	1874.92	J/mol×K	1130.03	Joback Method
cpg	1939.67	J/mol×K	1171.35	Joback Method
cpg	2010.34	J/mol×K	1212.68	Joback Method
cpg	2087.70	J/mol×K	1254.00	Joback Method
cpg	2172.47	J/mol×K	1295.32	Joback Method
cpg	2265.40	J/mol×K	1336.64	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=R110133&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