24-Methyl-7-lanosterol acetate

Inchi: InChI=1S/C33H54O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(3
InchiKey: BIJBAWUBTMORRK-DZPUZQRXSA-N
Formula: C33H54O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(C(C)CCC(C)=C(C)C)CCC4(C)C3=CCC2C1(C)C
Mol. weight [g/mol]: 482.78

Physical Properties

Property code	Value	Unit	Source
gf	203.77	kJ/mol	Joback Method
hf	-590.58	kJ/mol	Joback Method
hfus	40.04	kJ/mol	Joback Method
hvap	93.56	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.296		Crippen Method
mcvol	431.230	ml/mol	McGowan Method
pc	790.82	kPa	Joback Method
rinpol	3449.00		NIST Webbook
tb	1068.94	K	Joback Method
tc	1312.86	K	Joback Method
tf	631.91	K	Joback Method
vc	1.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1733.70	J/mol×K	1068.94	Joback Method
cpg	1789.06	J/mol×K	1109.59	Joback Method
cpg	1848.92	J/mol×K	1150.25	Joback Method
cpg	1913.96	J/mol×K	1190.90	Joback Method
cpg	1984.85	J/mol×K	1231.56	Joback Method
cpg	2062.28	J/mol×K	1272.21	Joback Method
cpg	2146.90	J/mol×K	1312.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110460&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