24-Methylene-24-dihydrolanosterol 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: XJAUCFFDVQSSEW-UHFFFAOYSA-N
Formula: C33H54O2
SMILES: C=C(CCC(C)C1CCC2(C)C3=C(CCC12C)C1(C)CCC(OC(C)=O)C(C)(C)C1CC3)C(C)C
Mol. weight [g/mol]: 482.78
CAS: 17837-80-8

Physical Properties

Property code	Value	Unit	Source
gf	215.58	kJ/mol	Joback Method
hf	-568.99	kJ/mol	Joback Method
hfus	34.88	kJ/mol	Joback Method
hvap	93.44	kJ/mol	Joback Method
log10ws	-9.96		Crippen Method
logp	9.296		Crippen Method
mcvol	431.230	ml/mol	McGowan Method
pc	795.73	kPa	Joback Method
rinpol	3391.00		NIST Webbook
tb	1070.79	K	Joback Method
tc	1314.23	K	Joback Method
tf	650.95	K	Joback Method
vc	1.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1728.47	J/mol×K	1070.79	Joback Method
cpg	1783.32	J/mol×K	1111.36	Joback Method
cpg	1842.61	J/mol×K	1151.94	Joback Method
cpg	1906.99	J/mol×K	1192.51	Joback Method
cpg	1977.12	J/mol×K	1233.09	Joback Method
cpg	2053.66	J/mol×K	1273.66	Joback Method
cpg	2137.28	J/mol×K	1314.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17837808&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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