24-Methyl-24-dihydrolanosterol acetate

Inchi: InChI=1S/C33H56O2/c1-21(2)22(3)11-12-23(4)25-15-19-33(10)27-13-14-28-30(6,7)29(3
InchiKey: SWYDFFCKOFIWAM-LXOXAYJKSA-N
Formula: C33H56O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC(C(C)CCC(C)C(C)C)C1(C)CC3
Mol. weight [g/mol]: 484.80

Physical Properties

Property code	Value	Unit	Source
gf	133.85	kJ/mol	Joback Method
hf	-689.91	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	93.64	kJ/mol	Joback Method
log10ws	-9.87		Crippen Method
logp	9.376		Crippen Method
mcvol	435.530	ml/mol	McGowan Method
pc	778.51	kPa	Joback Method
rinpol	3397.00		NIST Webbook
rinpol	3397.00		NIST Webbook
tb	1073.79	K	Joback Method
tc	1316.91	K	Joback Method
tf	651.67	K	Joback Method
vc	1.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1762.30	J/mol×K	1073.79	Joback Method
cpg	1817.52	J/mol×K	1114.31	Joback Method
cpg	1877.07	J/mol×K	1154.83	Joback Method
cpg	1941.59	J/mol×K	1195.35	Joback Method
cpg	2011.74	J/mol×K	1235.87	Joback Method
cpg	2088.15	J/mol×K	1276.39	Joback Method
cpg	2171.49	J/mol×K	1316.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110391&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