23,24-Dimethyl-5,22-cholestadienol acetate

Inchi: InChI=1S/C31H50O2/c1-19(2)22(5)20(3)17-21(4)27-11-12-28-26-10-9-24-18-25(33-23(6)
InchiKey: WSZYWDNSBDPRRZ-SAJCIRDNSA-N
Formula: C31H50O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)C=C(C)C(C)C(C)C)CCC32)C1
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	209.29	kJ/mol	Joback Method
hf	-560.21	kJ/mol	Joback Method
hfus	40.65	kJ/mol	Joback Method
hvap	90.87	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.372		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	859.99	kPa	Joback Method
rinpol	3297.00		NIST Webbook
rinpol	3297.00		NIST Webbook
tb	1026.61	K	Joback Method
tc	1264.27	K	Joback Method
tf	549.77	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1548.78	J/mol×K	1026.61	Joback Method
cpg	1584.71	J/mol×K	1066.22	Joback Method
cpg	1621.76	J/mol×K	1105.83	Joback Method
cpg	1660.33	J/mol×K	1145.44	Joback Method
cpg	1700.84	J/mol×K	1185.05	Joback Method
cpg	1743.68	J/mol×K	1224.66	Joback Method
cpg	1789.24	J/mol×K	1264.27	Joback Method

Sources

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=R110108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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