23-Demethylgorgosterol acetate

Inchi: InChI=1S/C31H50O2/c1-18(2)19(3)25-17-26(25)20(4)27-10-11-28-24-9-8-22-16-23(33-2
InchiKey: XERVJQNPZBDWNL-ITNQQFKJSA-N
Formula: C31H50O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)C4CC4C(C)C(C)C)CCC32)C1
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	190.66	kJ/mol	Joback Method
hf	-615.18	kJ/mol	Joback Method
hfus	40.96	kJ/mol	Joback Method
hvap	90.43	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	8.061		Crippen Method
mcvol	396.490	ml/mol	McGowan Method
pc	880.52	kPa	Joback Method
rinpol	3369.00		NIST Webbook
tb	1024.64	K	Joback Method
tc	1262.80	K	Joback Method
tf	582.51	K	Joback Method
vc	1.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1564.57	J/mol×K	1024.64	Joback Method
cpg	1601.00	J/mol×K	1064.33	Joback Method
cpg	1638.50	J/mol×K	1104.03	Joback Method
cpg	1677.50	J/mol×K	1143.72	Joback Method
cpg	1718.41	J/mol×K	1183.41	Joback Method
cpg	1761.64	J/mol×K	1223.11	Joback Method
cpg	1807.61	J/mol×K	1262.80	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=R110128&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