Clerosterol acetate

Inchi: InChI=1S/C31H50O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
InchiKey: XSBVQWHCFJNQMD-WEZVYXGHSA-N
Formula: C31H50O2
SMILES: C=C(C)C(CC)CCC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	219.35	kJ/mol	Joback Method
hf	-546.72	kJ/mol	Joback Method
hfus	42.69	kJ/mol	Joback Method
hvap	90.63	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	8.516		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	850.98	kPa	Joback Method
rinpol	3343.00		NIST Webbook
tb	1019.57	K	Joback Method
tc	1253.53	K	Joback Method
tf	568.09	K	Joback Method
vc	1.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1543.88	J/mol×K	1019.57	Joback Method
cpg	1578.76	J/mol×K	1058.56	Joback Method
cpg	1614.57	J/mol×K	1097.56	Joback Method
cpg	1651.67	J/mol×K	1136.55	Joback Method
cpg	1690.45	J/mol×K	1175.54	Joback Method
cpg	1731.26	J/mol×K	1214.53	Joback Method
cpg	1774.49	J/mol×K	1253.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R87487&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