5,22,25-Stigmastatrienol acetate

Inchi: InChI=1S/C31H48O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
InchiKey: MOEVEIGHSLNJAI-APVDANIJSA-N
Formula: C31H48O2
SMILES: C=C(C)C(C=CC(C)C1CCC2C3CC=C4CC(OC(C)=O)CCC4(C)C3CCC12C)CC
Mol. weight [g/mol]: 452.71

Physical Properties

Property code	Value	Unit	Source
gf	299.57	kJ/mol	Joback Method
hf	-429.50	kJ/mol	Joback Method
hfus	42.89	kJ/mol	Joback Method
hvap	90.58	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	8.292		Crippen Method
mcvol	398.750	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	3305.00		NIST Webbook
rinpol	3305.00		NIST Webbook
tb	1023.73	K	Joback Method
tc	1261.05	K	Joback Method
tf	563.01	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1516.89	J/mol×K	1023.73	Joback Method
cpg	1552.36	J/mol×K	1063.28	Joback Method
cpg	1589.04	J/mol×K	1102.84	Joback Method
cpg	1627.34	J/mol×K	1142.39	Joback Method
cpg	1667.65	J/mol×K	1181.94	Joback Method
cpg	1710.39	J/mol×K	1221.50	Joback Method
cpg	1755.98	J/mol×K	1261.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110757&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

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