Stigmastanol acetate

Inchi: InChI=1S/C31H54O2/c1-8-23(20(2)3)10-9-21(4)27-13-14-28-26-12-11-24-19-25(33-22(5
InchiKey: UOLJGJFAVGOXAH-OMJQXHSWSA-N
Formula: C31H54O2
SMILES: CCC(CCC(C)C1CCC2C3CCC4CC(OC(C)=O)CCC4(C)C3CCC12C)C(C)C
Mol. weight [g/mol]: 458.76

Physical Properties

Property code	Value	Unit	Source
gf	109.58	kJ/mol	Joback Method
hf	-734.29	kJ/mol	Joback Method
hfus	41.99	kJ/mol	Joback Method
hvap	89.57	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	8.675		Crippen Method
mcvol	411.650	ml/mol	McGowan Method
pc	806.62	kPa	Joback Method
rinpol	3369.00		NIST Webbook
tb	1013.76	K	Joback Method
tc	1245.17	K	Joback Method
tf	551.29	K	Joback Method
vc	1.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1609.44	J/mol×K	1013.76	Joback Method
cpg	1644.72	J/mol×K	1052.33	Joback Method
cpg	1680.59	J/mol×K	1090.90	Joback Method
cpg	1717.39	J/mol×K	1129.46	Joback Method
cpg	1755.47	J/mol×K	1168.03	Joback Method
cpg	1795.20	J/mol×K	1206.60	Joback Method
cpg	1836.91	J/mol×K	1245.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R8596&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