5,23-Ergostadienol acetate

Inchi: InChI=1S/C30H48O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31)
InchiKey: FPNGSVYWFLQCOM-YBEYRSLXSA-N
Formula: C30H48O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3C2CCC2(C)C(C(C)CC=C(C)C(C)C)CCC32)C1
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	203.31	kJ/mol	Joback Method
hf	-534.29	kJ/mol	Joback Method
hfus	41.58	kJ/mol	Joback Method
hvap	89.03	kJ/mol	Joback Method
log10ws	-8.71		Crippen Method
logp	8.126		Crippen Method
mcvol	388.960	ml/mol	McGowan Method
pc	906.15	kPa	Joback Method
rinpol	3269.00		NIST Webbook
rinpol	3269.00		NIST Webbook
tb	1004.17	K	Joback Method
tc	1239.29	K	Joback Method
tf	553.50	K	Joback Method
vc	1.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1476.56	J/mol×K	1004.17	Joback Method
cpg	1510.91	J/mol×K	1043.36	Joback Method
cpg	1546.20	J/mol×K	1082.54	Joback Method
cpg	1582.81	J/mol×K	1121.73	Joback Method
cpg	1621.13	J/mol×K	1160.92	Joback Method
cpg	1661.55	J/mol×K	1200.10	Joback Method
cpg	1704.46	J/mol×K	1239.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110762&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