5,8,22-Ergostatrienol acetate

Inchi: InChI=1S/C30H46O2/c1-19(2)20(3)8-9-21(4)26-12-13-27-25-11-10-23-18-24(32-22(5)31)
InchiKey: PHJBQRYRTHXDED-KNNMHKCVSA-N
Formula: C30H46O2
SMILES: CC(=O)OC1CCC2(C)C(=CCC3=C2CCC2(C)C3CCC2C(C)C=CC(C)C(C)C)C1
Mol. weight [g/mol]: 438.69

Physical Properties

Property code	Value	Unit	Source
gf	235.54	kJ/mol	Joback Method
hf	-454.26	kJ/mol	Joback Method
hfus	37.67	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	8.046		Crippen Method
mcvol	384.660	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	3246.00		NIST Webbook
tb	1022.31	K	Joback Method
tc	1260.96	K	Joback Method
tf	586.74	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1442.05	J/mol×K	1022.31	Joback Method
cpg	1476.72	J/mol×K	1062.09	Joback Method
cpg	1512.73	J/mol×K	1101.86	Joback Method
cpg	1550.51	J/mol×K	1141.64	Joback Method
cpg	1590.46	J/mol×K	1181.41	Joback Method
cpg	1632.98	J/mol×K	1221.19	Joback Method
cpg	1678.48	J/mol×K	1260.96	Joback Method

Sources

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=R110826&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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