Vernosterol acetate

Inchi: InChI=1S/C30H46O2/c1-8-22(19(2)3)17-20(4)26-11-12-27-25-10-9-23-18-24(32-21(5)31)
InchiKey: ORZLNKKIYBRHAR-ZMFSMEMUSA-N
Formula: C30H46O2
SMILES: CC=C(CC(C)C1CC=C2C3=C(CCC21C)C1(C)CCC(OC(C)=O)CC1CC3)C(C)C
Mol. weight [g/mol]: 438.69

Physical Properties

Property code	Value	Unit	Source
gf	229.43	kJ/mol	Joback Method
hf	-458.77	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	91.26	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.190		Crippen Method
mcvol	384.660	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	3385.00		NIST Webbook
rinpol	3385.00		NIST Webbook
tb	1022.63	K	Joback Method
tc	1261.04	K	Joback Method
tf	587.78	K	Joback Method
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.58	J/mol×K	1022.63	Joback Method
cpg	1476.36	J/mol×K	1062.37	Joback Method
cpg	1512.51	J/mol×K	1102.10	Joback Method
cpg	1550.45	J/mol×K	1141.84	Joback Method
cpg	1590.58	J/mol×K	1181.57	Joback Method
cpg	1633.31	J/mol×K	1221.31	Joback Method
cpg	1679.04	J/mol×K	1261.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R111498&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