24-Dihydrotirucallol acetate

Inchi: InChI=1S/C32H54O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-23
InchiKey: VARRUGKCHMYWET-JPOUBOMKSA-N
Formula: C32H54O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC(C(C)CCCC(C)C)C1(C)CC3
Mol. weight [g/mol]: 470.77

Physical Properties

Property code	Value	Unit	Source
gf	127.87	kJ/mol	Joback Method
hf	-663.99	kJ/mol	Joback Method
hfus	34.88	kJ/mol	Joback Method
hvap	91.80	kJ/mol	Joback Method
log10ws	-9.69		Crippen Method
logp	9.130		Crippen Method
mcvol	421.440	ml/mol	McGowan Method
pc	818.20	kPa	Joback Method
rinpol	3291.00		NIST Webbook
tb	1051.35	K	Joback Method
tc	1290.99	K	Joback Method
tf	655.40	K	Joback Method
vc	1.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1680.25	J/mol×K	1051.35	Joback Method
cpg	1731.90	J/mol×K	1091.29	Joback Method
cpg	1787.46	J/mol×K	1131.23	Joback Method
cpg	1847.54	J/mol×K	1171.17	Joback Method
cpg	1912.77	J/mol×K	1211.11	Joback Method
cpg	1983.75	J/mol×K	1251.05	Joback Method
cpg	2061.12	J/mol×K	1290.99	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110262&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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