Tirucallol acetate

Inchi: InChI=1S/C32H52O2/c1-21(2)11-10-12-22(3)24-15-19-32(9)26-13-14-27-29(5,6)28(34-23
InchiKey: BQPPJGMMIYJVBR-NUBGRVATSA-N
Formula: C32H52O2
SMILES: CC(=O)OC1CCC2(C)C3=C(CCC2C1(C)C)C1(C)CCC(C(C)CCC=C(C)C)C1(C)CC3
Mol. weight [g/mol]: 468.75
CAS: 52689-37-9

Physical Properties

Property code	Value	Unit	Source
gf	201.98	kJ/mol	Joback Method
hf	-551.28	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-9.79		Crippen Method
logp	9.050		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	841.62	kPa	Joback Method
rinpol	3323.00		NIST Webbook
tb	1055.83	K	Joback Method
tc	1298.35	K	Joback Method
tf	651.36	K	Joback Method
vc	1.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1654.54	J/mol×K	1055.83	Joback Method
cpg	1707.58	J/mol×K	1096.25	Joback Method
cpg	1764.97	J/mol×K	1136.67	Joback Method
cpg	1827.36	J/mol×K	1177.09	Joback Method
cpg	1895.41	J/mol×K	1217.51	Joback Method
cpg	1969.79	J/mol×K	1257.93	Joback Method
cpg	2051.14	J/mol×K	1298.35	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=C52689379&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