24-Methyl-23-dehydrolophenol acetate

Inchi: InChI=1S/C31H50O2/c1-19(2)20(3)9-10-21(4)25-13-14-27-24-11-12-26-22(5)29(33-23(6)
InchiKey: ORXXECLZMPJQFD-NGGGMAIESA-N
Formula: C31H50O2
SMILES: CC(=O)OC1CCC2(C)C3CCC4(C)C(CCC4C(C)CC=C(C)C(C)C)C3=CCC2C1C
Mol. weight [g/mol]: 454.73

Physical Properties

Property code	Value	Unit	Source
gf	204.02	kJ/mol	Joback Method
hf	-575.27	kJ/mol	Joback Method
hfus	45.24	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	8.372		Crippen Method
mcvol	403.050	ml/mol	McGowan Method
pc	839.67	kPa	Joback Method
rinpol	3364.00		NIST Webbook
tb	1022.38	K	Joback Method
tc	1258.09	K	Joback Method
tf	560.53	K	Joback Method
vc	1.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1551.14	J/mol×K	1022.38	Joback Method
cpg	1586.65	J/mol×K	1061.66	Joback Method
cpg	1623.13	J/mol×K	1100.95	Joback Method
cpg	1660.96	J/mol×K	1140.23	Joback Method
cpg	1700.53	J/mol×K	1179.52	Joback Method
cpg	1742.21	J/mol×K	1218.80	Joback Method
cpg	1786.39	J/mol×K	1258.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110371&Units=SI

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