24-Ethyl-24(25)-dehydrolophenol acetate

Inchi: InChI=1S/C32H52O2/c1-9-24(20(2)3)11-10-21(4)26-14-15-28-25-12-13-27-22(5)30(34-2
InchiKey: DOWCXOIMGHTLGU-WAMVFHDGSA-N
Formula: C32H52O2
SMILES: CCC(CCC(C)C1CCC2C3=CCC4C(C)C(OC(C)=O)CCC4(C)C3CCC21C)=C(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	206.33	kJ/mol	Joback Method
hf	-600.42	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	93.64	kJ/mol	Joback Method
log10ws	-9.54		Crippen Method
logp	8.906		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	793.49	kPa	Joback Method
rinpol	3491.00		NIST Webbook
rinpol	3491.00		NIST Webbook
tb	1045.58	K	Joback Method
tc	1283.17	K	Joback Method
tf	572.84	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1623.90	J/mol×K	1045.58	Joback Method
cpg	1661.15	J/mol×K	1085.18	Joback Method
cpg	1699.60	J/mol×K	1124.78	Joback Method
cpg	1739.64	J/mol×K	1164.37	Joback Method
cpg	1781.67	J/mol×K	1203.97	Joback Method
cpg	1826.08	J/mol×K	1243.57	Joback Method
cpg	1873.27	J/mol×K	1283.17	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=R110306&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