24-Ethyl-23-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: ICFGLGPOODJPDO-YRYILIIBSA-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	212.44	kJ/mol	Joback Method
hf	-595.91	kJ/mol	Joback Method
hfus	47.83	kJ/mol	Joback Method
hvap	93.17	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	8.762		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	794.84	kPa	Joback Method
rinpol	3435.00		NIST Webbook
rinpol	3435.00		NIST Webbook
tb	1045.26	K	Joback Method
tc	1282.96	K	Joback Method
tf	571.80	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1624.27	J/mol×K	1045.26	Joback Method
cpg	1661.39	J/mol×K	1084.88	Joback Method
cpg	1699.67	J/mol×K	1124.49	Joback Method
cpg	1739.51	J/mol×K	1164.11	Joback Method
cpg	1781.31	J/mol×K	1203.73	Joback Method
cpg	1825.47	J/mol×K	1243.34	Joback Method
cpg	1872.38	J/mol×K	1282.96	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=R110297&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