24-Ethyl-25-dehydrolophenol acetate, 24-«beta»

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: UACMKUJYWHZEHR-GBSVDFTQSA-N
Formula: C32H52O2
SMILES: C=C(C)C(CC)CCC(C)C1CCC2C3=CCC4C(C)C(OC(C)=O)CCC4(C)C3CCC21C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	220.06	kJ/mol	Joback Method
hf	-587.70	kJ/mol	Joback Method
hfus	46.35	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	8.762		Crippen Method
mcvol	417.140	ml/mol	McGowan Method
pc	790.37	kPa	Joback Method
rinpol	3439.00		NIST Webbook
tb	1037.78	K	Joback Method
tc	1273.34	K	Joback Method
tf	575.12	K	Joback Method
vc	1.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1619.08	J/mol×K	1037.78	Joback Method
cpg	1655.22	J/mol×K	1077.04	Joback Method
cpg	1692.31	J/mol×K	1116.30	Joback Method
cpg	1730.74	J/mol×K	1155.56	Joback Method
cpg	1770.87	J/mol×K	1194.82	Joback Method
cpg	1813.08	J/mol×K	1234.08	Joback Method
cpg	1857.75	J/mol×K	1273.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R110311&Units=SI
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

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