labd-13(E)-en-8«alpha»-ol-15-yl acetate

Inchi: InChI=1S/C22H38O3/c1-16(11-15-25-17(2)23)8-9-19-21(5)13-7-12-20(3,4)18(21)10-14-2
InchiKey: GYGSQPMBVQQYCF-KIJIRQTNSA-N
Formula: C22H38O3
SMILES: CC(=O)OCC=C(C)CCC1C(C)(O)CCC2C(C)(C)CCCC21C
Mol. weight [g/mol]: 350.54

Physical Properties

Property code	Value	Unit	Source
gf	-131.21	kJ/mol	Joback Method
hf	-681.35	kJ/mol	Joback Method
hfus	30.69	kJ/mol	Joback Method
hvap	86.57	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	5.270		Crippen Method
mcvol	308.130	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2505.00		NIST Webbook
tb	892.54	K	Joback Method
tc	1106.46	K	Joback Method
tf	532.42	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1074.45	J/mol×K	892.54	Joback Method
cpg	1101.34	J/mol×K	928.19	Joback Method
cpg	1129.02	J/mol×K	963.85	Joback Method
cpg	1157.81	J/mol×K	999.50	Joback Method
cpg	1188.00	J/mol×K	1035.15	Joback Method
cpg	1219.92	J/mol×K	1070.80	Joback Method
cpg	1253.86	J/mol×K	1106.46	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=R327678&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