labd-7,13(E)-dien-15-yl acetate

Inchi: InChI=1S/C22H36O2/c1-16(12-15-24-18(3)23)8-10-19-17(2)9-11-20-21(4,5)13-7-14-22(1
InchiKey: DEKPALIRJFSIQW-ZPUHZNKNSA-N
Formula: C22H36O2
SMILES: CC(=O)OCC=C(C)CCC1C(C)=CCC2C(C)(C)CCCC12C
Mol. weight [g/mol]: 332.52

Physical Properties

Property code	Value	Unit	Source
gf	39.14	kJ/mol	Joback Method
hf	-477.71	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	72.31	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	6.075		Crippen Method
mcvol	297.960	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2393.00		NIST Webbook
ripol	2561.00		NIST Webbook
tb	808.93	K	Joback Method
tc	1025.15	K	Joback Method
tf	465.22	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.34	J/mol×K	808.93	Joback Method
cpg	987.72	J/mol×K	844.97	Joback Method
cpg	1011.72	J/mol×K	881.00	Joback Method
cpg	1035.57	J/mol×K	917.04	Joback Method
cpg	1059.52	J/mol×K	953.08	Joback Method
cpg	1083.79	J/mol×K	989.11	Joback Method
cpg	1108.62	J/mol×K	1025.15	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=R327698&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume