Lanceol acetate

Inchi: InChI=1S/C17H26O2/c1-13-8-10-17(11-9-13)15(3)7-5-6-14(2)12-19-16(4)18/h6,8,17H,3,
InchiKey: BSYWXGDMWUUHDZ-NSIKDUERSA-N
Formula: C17H26O2
SMILES: C=C(CCC=C(C)COC(C)=O)C1CC=C(C)CC1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
gf	54.08	kJ/mol	Joback Method
hf	-315.31	kJ/mol	Joback Method
hfus	31.54	kJ/mol	Joback Method
hvap	63.42	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.579		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
pc	1633.81	kPa	Joback Method
rinpol	1860.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1856.00		NIST Webbook
rinpol	1860.00		NIST Webbook
tb	688.94	K	Joback Method
tc	894.75	K	Joback Method
tf	339.41	K	Joback Method
vc	0.893	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.93	J/mol×K	688.94	Joback Method
cpg	677.21	J/mol×K	723.24	Joback Method
cpg	695.35	J/mol×K	757.54	Joback Method
cpg	712.40	J/mol×K	791.85	Joback Method
cpg	728.40	J/mol×K	826.15	Joback Method
cpg	743.40	J/mol×K	860.45	Joback Method

cpg	757.44	J/mol×K	894.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R331474&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