(-)-Isolongifolol, acetate

Inchi: InChI=1S/C17H28O2/c1-11(18)19-10-14-12-6-7-13-15(12)16(2,3)8-5-9-17(13,14)4/h12-1
InchiKey: FWCPQBUXTSVEIC-UHFFFAOYSA-N
Formula: C17H28O2
SMILES: CC(=O)OCC1C2CCC3C2C(C)(C)CCCC13C
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-17.72	kJ/mol	Joback Method
hf	-463.47	kJ/mol	Joback Method
hfus	23.39	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	4.038		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1850.30		NIST Webbook
rinpol	1850.30		NIST Webbook
tb	679.88	K	Joback Method
tc	898.50	K	Joback Method
tf	435.37	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.39	J/mol×K	679.88	Joback Method
cpg	717.09	J/mol×K	716.32	Joback Method
cpg	738.84	J/mol×K	752.75	Joback Method
cpg	759.91	J/mol×K	789.19	Joback Method
cpg	780.54	J/mol×K	825.63	Joback Method
cpg	801.00	J/mol×K	862.06	Joback Method
cpg	821.54	J/mol×K	898.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352280&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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