14-Acetoxy-4,5-dihydro- «beta»-caryophyllene

Inchi: InChI=1S/C17H28O2/c1-12-6-5-7-14(11-19-13(2)18)8-9-16-15(12)10-17(16,3)4/h14-16H
InchiKey: IUJQNPWRCLHBKE-UHFFFAOYSA-N
Formula: C17H28O2
SMILES: C=C1CCCC(COC(C)=O)CCC2C1CC2(C)C
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-48.49	kJ/mol	Joback Method
hf	-465.41	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.348		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1706.12	kPa	Joback Method
ripol	2282.00		NIST Webbook
ripol	2282.00		NIST Webbook
ripol	2282.00		NIST Webbook
tb	689.54	K	Joback Method
tc	908.30	K	Joback Method
tf	400.89	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.54	J/mol×K	689.54	Joback Method
cpg	718.66	J/mol×K	726.00	Joback Method
cpg	740.56	J/mol×K	762.46	Joback Method
cpg	761.34	J/mol×K	798.92	Joback Method
cpg	781.12	J/mol×K	835.38	Joback Method
cpg	800.01	J/mol×K	871.84	Joback Method
cpg	818.12	J/mol×K	908.30	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336137&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume