6-Acetoxy-«alpha»-humulene

Inchi: InChI=1S/C17H28O2/c1-13-8-9-16(19-15(3)18)14(2)7-6-11-17(4,5)12-10-13/h6,10-11,14
InchiKey: OOEIWBNDEFVSKN-PIUHNEHMSA-N
Formula: C17H28O2
SMILES: CC(=O)OC1CCC(C)=CCC(C)(C)C=CCC1C
Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	-148.33	kJ/mol	Joback Method
hf	-536.84	kJ/mol	Joback Method
hfus	21.81	kJ/mol	Joback Method
hvap	63.36	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.657		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	699.75	K	Joback Method
tc	927.49	K	Joback Method
tf	372.75	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.67	J/mol×K	699.75	Joback Method
cpg	720.71	J/mol×K	737.71	Joback Method
cpg	743.38	J/mol×K	775.66	Joback Method
cpg	764.73	J/mol×K	813.62	Joback Method
cpg	784.84	J/mol×K	851.58	Joback Method
cpg	803.78	J/mol×K	889.53	Joback Method
cpg	821.61	J/mol×K	927.49	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=R628783&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume