14-Acetoxy-«alpha»-humulene

Other names: 14-Hydroxy-«alpha»-humulene acetate
Inchi: InChI=1S/C17H26O2/c1-14-7-5-8-16(13-19-15(2)18)9-6-11-17(3,4)12-10-14/h6,8,10-11H
InchiKey: HRJAXTXFMJCTOQ-AOVTVKOZSA-N
Formula: C17H26O2
SMILES: CC(=O)OCC1=CCCC(C)=CCC(C)(C)C=CC1
Mol. weight [g/mol]: 262.39

Physical Properties

Property code	Value	Unit	Source
hfus	20.50	kJ/mol	Joback Method
ie	8.35	eV	Cheméo Relay (1.0)
logp	4.579		Crippen Method
mcvol	234.070	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2329.00		NIST Webbook
ripol	2329.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.14	J/mol×K	713.23	Joback Method
cpg	690.01	J/mol×K	751.62	Joback Method
cpg	710.63	J/mol×K	790.01	Joback Method
cpg	730.10	J/mol×K	828.39	Joback Method
cpg	748.50	J/mol×K	866.78	Joback Method
cpg	765.91	J/mol×K	905.17	Joback Method
cpg	782.41	J/mol×K	943.56	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R336117&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices