14-Hydroxy-«alpha»-humulene, coumarate

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	3153.00		NIST Webbook
rinpol	3153.00		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

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R628763&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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