6-Hydroxy-«alpha»-humulene

Inchi: InChI=1S/C15H26O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h5,9-10,13-14,16H,6-8
InchiKey: JXLVPCWSMFUWOE-VKLURXMVSA-N
Formula: C15H26O
SMILES: CC1=CCC(C)(C)C=CCC(C)C(O)CC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
hfus	17.93	kJ/mol	Joback Method
ie	8.56	eV	Cheméo Relay (1.0)
logp	4.086		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
rinpol	1656.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.52	J/mol×K	669.88	Joback Method
cpg	621.01	J/mol×K	705.71	Joback Method
cpg	641.36	J/mol×K	741.55	Joback Method
cpg	660.64	J/mol×K	777.38	Joback Method
cpg	678.92	J/mol×K	813.22	Joback Method
cpg	696.28	J/mol×K	849.05	Joback Method
cpg	712.77	J/mol×K	884.88	Joback Method

Sources

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=R628798&Units=SI
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
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