(6R)-Hydroxy-«alpha»-humulene

Inchi: InChI=1S/C15H24O/c1-12-7-8-14(16)13(2)6-5-10-15(3,4)11-9-12/h5,9-10,14,16H,2,6-8,1
InchiKey: ZHCPVYWHSOILQL-IGORNAHMSA-N
Formula: C15H24O
SMILES: C=C1CC=CC(C)(C)CC=C(C)CCC1O
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
hfus	15.70	kJ/mol	Joback Method
ie	8.54	eV	Cheméo Relay (1.0)
logp	4.006		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
rinpol	1657.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.42	J/mol×K	673.71	Joback Method
cpg	593.46	J/mol×K	709.82	Joback Method
cpg	612.44	J/mol×K	745.92	Joback Method
cpg	630.44	J/mol×K	782.03	Joback Method
cpg	647.51	J/mol×K	818.13	Joback Method
cpg	663.75	J/mol×K	854.24	Joback Method
cpg	679.22	J/mol×K	890.35	Joback Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R618974&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