

14-Hydroxy-«alpha»-humulene

Inchi:	InChI=1S/C15H24O/c1-13-6-4-7-14(12-16)8-5-10-15(2,3)11-9-13/h5,7,9-10,16H,4,6,8,11
InchiKey:	BNIJVVJLOOJV DGU-ZMYZPJLPSA-N
Formula:	C15H24O
SMILES:	CC1=CCC(C)(C)C=CCC(CO)=CCC1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	-32.32	kJ/mol	Joback Method
hf	-316.00	kJ/mol	Joback Method
hfus	16.62	kJ/mol	Joback Method
hvap	68.00	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	4.008		Crippen Method
mcvol	204.320	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
rinpola	1780.00		NIST Webbook
ripola	2378.00		NIST Webbook
tb	683.36	K	Joback Method
tc	901.01	K	Joback Method
tf	360.63	K	Joback Method
vc	0.744	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.12	J/mol×K	683.36	Joback Method
cpg	591.49	J/mol×K	719.64	Joback Method
cpg	609.84	J/mol×K	755.91	Joback Method
cpg	627.25	J/mol×K	792.19	Joback Method
cpg	643.82	J/mol×K	828.46	Joback Method
cpg	659.61	J/mol×K	864.74	Joback Method
cpg	674.72	J/mol×K	901.01	Joback Method

Sources

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=R611933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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