

14-Hydroxy-«alpha»-humulene

Other names:	«alpha»-Humulene, 14-hydroxy-Humulene (14-hydroxy- «alpha»)
Inchi:	InChI=1S/C15H24O/c1-13-6-4-7-14(2)9-11-15(3,12-16)10-5-8-13/h5-6,9-10,16H,4,7-8,11
InchiKey:	YLOBZQJVNNUEPZ-NYAJVKMDSA-N
Formula:	C15H24O
SMILES:	CC1=CCCC(C)=CCC(C)(CO)C=CC1
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
rinpol	1703.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1709.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1718.00		NIST Webbook
ripol	2478.00		NIST Webbook
ripol	2478.00		NIST Webbook
ripol	2478.00		NIST Webbook
ripol	2478.00		NIST Webbook
ripol	2475.00		NIST Webbook
tb	683.36	K	Joback Method
tc	901.01	K	Joback Method
tf	360.63	K	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R199998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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