

Humulane

Inchi:	InChI=1S/C15H30/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h13-14H,5-12H2,1-4H3
InchiKey:	UTJJFHJHTZKQSW-UHFFFAOYSA-N
Formula:	C15H30
SMILES:	CC1CCCC(C)CCC(C)(C)CCC1
Mol. weight [g/mol]:	210.40

Physical Properties

Property code	Value	Unit	Source
gf	18.46	kJ/mol	Joback Method
hf	-354.85	kJ/mol	Joback Method
hfus	11.78	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	5.419		Crippen Method
mcvol	211.350	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
ripol	1521.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1609.00		NIST Webbook
ripol	1637.00		NIST Webbook
tb	574.40	K	Joback Method
tc	802.23	K	Joback Method
tf	264.01	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.72	J/molxK	574.40	Joback Method
cpg	589.76	J/molxK	612.37	Joback Method
cpg	617.15	J/molxK	650.34	Joback Method
cpg	642.99	J/molxK	688.32	Joback Method
cpg	667.37	J/molxK	726.29	Joback Method

cpg	690.37	J/mol×K	764.26	Joback Method
cpg	712.09	J/mol×K	802.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R207757&Units=SI

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

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