

Tetrahydrohumulene

Inchi:	InChI=1S/C15H28/c1-13-7-5-8-14(2)10-12-15(3,4)11-6-9-13/h6,11,13-14H,5,7-10,12H2,1
InchiKey:	DAQZJCXSMVNPBE-IZZDOVSWSA-N
Formula:	C15H28
SMILES:	CC1CC=CC(C)(C)CCC(C)CCC1
Mol. weight [g/mol]:	208.38

Physical Properties

Property code	Value	Unit	Source
gf	48.42	kJ/mol	Joback Method
hf	-297.07	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	48.80	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	5.195		Crippen Method
mcvol	207.050	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1523.00		NIST Webbook
rinpol	1504.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1653.00		NIST Webbook
ripol	1653.00		NIST Webbook
tb	573.56	K	Joback Method
tc	803.64	K	Joback Method
tf	264.77	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.70	J/mol×K	573.56	Joback Method
cpg	568.65	J/mol×K	611.91	Joback Method
cpg	594.99	J/mol×K	650.25	Joback Method
cpg	619.80	J/mol×K	688.60	Joback Method

cpg	643.18	J/mol×K	726.95	Joback Method
cpg	665.23	J/mol×K	765.29	Joback Method
cpg	686.04	J/mol×K	803.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R207762&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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