

Humulol

Other names:	(3E,7E)-1,5,5,8-Tetramethylcycloundeca-3,7-dienol
Inchi:	InChI=1S/C15H26O/c1-13-7-5-10-15(4,16)11-6-9-14(2,3)12-8-13/h6,8-9,16H,5,7,10-12H
InchiKey:	ZLMAVMBYWKVCLV-IMWXLZLDSA-N
Formula:	C15H26O
SMILES:	CC1=CCC(C)(C)C=CCC(C)(O)CCC1
Mol. weight [g/mol]:	222.37
CAS:	28446-26-6

Physical Properties

Property code	Value	Unit	Source
gf	-65.85	kJ/mol	Joback Method
hf	-367.41	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1618.00		NIST Webbook
rinpol	1609.90		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1609.90		NIST Webbook
ripol	2124.00		NIST Webbook
ripol	2124.00		NIST Webbook
tb	674.79	K	Joback Method
tc	897.41	K	Joback Method
tf	367.01	K	Joback Method
vc	0.754	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.94	J/molxK	674.79	Joback Method
cpg	615.03	J/molxK	711.89	Joback Method

cpg	635.21	J/mol×K	749.00	Joback Method
cpg	654.65	J/mol×K	786.10	Joback Method
cpg	673.53	J/mol×K	823.20	Joback Method
cpg	692.04	J/mol×K	860.30	Joback Method
cpg	710.36	J/mol×K	897.41	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C28446266&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
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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