

# 2-Hexyne, 5,5-dimethyl

Inchi:	InChI=1S/C8H14/c1-5-6-7-8(2,3)4/h7H2,1-4H3
InchiKey:	AXLFTJMZKJKQIK-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	CC#CCC(C)(C)C
Mol. weight [g/mol]:	110.20
CAS:	56617-18-6

## Physical Properties

Property code	Value	Unit	Source
gf	222.12	kJ/mol	Joback Method
hf	55.10	kJ/mol	Joback Method
hfus	12.18	kJ/mol	Joback Method
hvap	34.26	kJ/mol	Joback Method
ie	9.28 ± 0.01	eV	NIST Webbook
log10ws	-2.72		Crippen Method
logp	2.446		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	740.00		NIST Webbook
rinpol	740.00		NIST Webbook
tb	388.21	K	Joback Method
tc	588.56	K	Joback Method
tf	288.44	K	Joback Method
vc	0.434	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.81	J/mol×K	388.21	Joback Method
cpg	223.46	J/mol×K	421.60	Joback Method
cpg	236.39	J/mol×K	454.99	Joback Method
cpg	248.63	J/mol×K	488.38	Joback Method
cpg	260.22	J/mol×K	521.78	Joback Method
cpg	271.19	J/mol×K	555.17	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C56617186&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C56617186&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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