

# 2-Hexyne, 4,5-dimethyl

<b>Inchi:</b>	InChI=1S/C8H14/c1-5-6-8(4)7(2)3/h7-8H,1-4H3
<b>InchiKey:</b>	DFMQGJKNWBUODK-UHFFFAOYSA-N
<b>Formula:</b>	C8H14
<b>SMILES:</b>	CC#CC(C)C(C)C
<b>Mol. weight [g/mol]:</b>	110.20

## Physical Properties

Property code	Value	Unit	Source
gf	214.40	kJ/mol	Joback Method
hf	53.29	kJ/mol	Joback Method
hfus	12.55	kJ/mol	Joback Method
hvap	34.78	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.302		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
rinpol	760.00		NIST Webbook
rinpol	760.00		NIST Webbook
tb	390.56	K	Joback Method
tc	587.09	K	Joback Method
tf	256.02	K	Joback Method
vc	0.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.27	J/mol×K	390.56	Joback Method
cpg	221.10	J/mol×K	423.31	Joback Method
cpg	233.40	J/mol×K	456.07	Joback Method
cpg	245.18	J/mol×K	488.82	Joback Method
cpg	256.46	J/mol×K	521.58	Joback Method
cpg	267.24	J/mol×K	554.33	Joback Method
cpg	277.55	J/mol×K	587.09	Joback Method

# Sources

<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=R66586&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R66586&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</b>	Enthalpy of vaporization at standard conditions
<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>r in pol:</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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