

# 1-Hexyne, 3,4-dimethyl

Inchi:	InChI=1S/C8H14/c1-5-7(3)8(4)6-2/h1,7-8H,6H2,2-4H3
InchiKey:	GYXPVYPQOHEKON-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	C#CC(C)C(C)CC
Mol. weight [g/mol]:	110.20

## Physical Properties

Property code	Value	Unit	Source
gf	234.67	kJ/mol	Joback Method
hf	72.89	kJ/mol	Joback Method
hfus	12.40	kJ/mol	Joback Method
hvap	32.48	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.302		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	3012.33	kPa	Joback Method
rinpola	727.00		NIST Webbook
rinpola	727.00		NIST Webbook
tb	371.68	K	Joback Method
tc	555.16	K	Joback Method
tf	196.89	K	Joback Method
vc	0.433	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.48	J/mol×K	371.68	Joback Method
cpg	219.93	J/mol×K	402.26	Joback Method
cpg	231.83	J/mol×K	432.84	Joback Method
cpg	243.21	J/mol×K	463.42	Joback Method
cpg	254.08	J/mol×K	494.00	Joback Method
cpg	264.45	J/mol×K	524.58	Joback Method
cpg	274.35	J/mol×K	555.16	Joback Method

# Sources

<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=R66483&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R66483&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>

# 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>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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