

# 1-Heptyne, 4-methyl

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

## Physical Properties

Property code	Value	Unit	Source
gf	237.11	kJ/mol	Joback Method
hf	78.17	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	32.87	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.446		Crippen Method
mcvol	114.980	ml/mol	McGowan Method
pc	2986.06	kPa	Joback Method
rinpol	750.00		NIST Webbook
tb	372.12	K	Joback Method
tc	551.24	K	Joback Method
tf	211.89	K	Joback Method
vc	0.440	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	207.61	J/mol×K	372.12	Joback Method
cpg	219.67	J/mol×K	401.97	Joback Method
cpg	231.21	J/mol×K	431.83	Joback Method
cpg	242.26	J/mol×K	461.68	Joback Method
cpg	252.83	J/mol×K	491.54	Joback Method
cpg	262.93	J/mol×K	521.39	Joback Method
cpg	272.59	J/mol×K	551.24	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=R66447&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R66447&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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