

# 5-Hepten-1-yne, 6-methyl

<b>Inchi:</b>	InChI=1S/C8H12/c1-4-5-6-7-8(2)3/h1,7H,5-6H2,2-3H3
<b>InchiKey:</b>	UDNVVNDNOWKDGK-UHFFFAOYSA-N
<b>Formula:</b>	C8H12
<b>SMILES:</b>	C#CCCC=C(C)C
<b>Mol. weight [g/mol]:</b>	108.18
<b>CAS:</b>	22842-10-0

## Physical Properties

Property code	Value	Unit	Source
gf	311.22	kJ/mol	Joback Method
hf	190.88	kJ/mol	Joback Method
hfus	18.34	kJ/mol	Joback Method
hvap	33.30	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.366		Crippen Method
mcvol	110.680	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	376.60	K	Joback Method
tc	564.72	K	Joback Method
tf	207.85	K	Joback Method
vc	0.426	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.43	J/mol×K	376.60	Joback Method
cpg	205.12	J/mol×K	407.95	Joback Method
cpg	216.20	J/mol×K	439.31	Joback Method
cpg	226.70	J/mol×K	470.66	Joback Method
cpg	236.66	J/mol×K	502.01	Joback Method
cpg	246.09	J/mol×K	533.36	Joback Method
cpg	255.03	J/mol×K	564.72	Joback Method

# Sources

<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>
<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=C22842100&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22842100&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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