

# 5-Methyl-5-hexen-3-yn-2-ol

<b>Inchi:</b>	InChI=1S/C7H10O/c1-6(2)4-5-7(3)8/h7-8H,1H2,2-3H3
<b>InchiKey:</b>	WMFIGZRDWHYIOC-UHFFFAOYSA-N
<b>Formula:</b>	C7H10O
<b>SMILES:</b>	C=C(C)C#CC(C)O
<b>Mol. weight [g/mol]:</b>	110.15
<b>CAS:</b>	68017-33-4

## Physical Properties

Property code	Value	Unit	Source
gf	150.89	kJ/mol	Joback Method
hf	42.62	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	0.947		Crippen Method
mcvol	102.460	ml/mol	McGowan Method
pc	3990.60	kPa	Joback Method
tb	456.86	K	Joback Method
tc	649.53	K	Joback Method
tf	304.85	K	Joback Method
vc	0.385	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.22	J/molxK	456.86	Joback Method
cpg	210.41	J/molxK	488.97	Joback Method
cpg	219.17	J/molxK	521.08	Joback Method
cpg	227.52	J/molxK	553.19	Joback Method
cpg	235.47	J/molxK	585.31	Joback Method
cpg	243.05	J/molxK	617.42	Joback Method
cpg	250.26	J/molxK	649.53	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=C68017334&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C68017334&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>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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