

# 3-Hexen-2-one, 4-hydroxy-5-methyl-

<b>Inchi:</b>	InChI=1S/C7H12O2/c1-5(2)7(9)4-6(3)8/h4-5,9H,1-3H3/b7-4-
<b>InchiKey:</b>	UTTSDKCNJMWXSK-DAXSKMNVSA-N
<b>Formula:</b>	C7H12O2
<b>SMILES:</b>	CC(=O)C=C(O)C(C)C
<b>Mol. weight [g/mol]:</b>	128.17
<b>CAS:</b>	35113-29-2

## Physical Properties

Property code	Value	Unit	Source
gf	-188.45	kJ/mol	Joback Method
hf	-350.47	kJ/mol	Joback Method
hfus	14.94	kJ/mol	Joback Method
hvap	54.25	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.673		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
tb	509.21	K	Joback Method
tc	693.39	K	Joback Method
tf	245.36	K	Joback Method
vc	0.427	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.70	J/molxK	509.21	Joback Method
cpg	257.54	J/molxK	539.91	Joback Method
cpg	266.88	J/molxK	570.60	Joback Method
cpg	275.76	J/molxK	601.30	Joback Method
cpg	284.19	J/molxK	632.00	Joback Method
cpg	292.18	J/molxK	662.69	Joback Method
cpg	299.77	J/molxK	693.39	Joback Method

# Sources

<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=C35113292&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35113292&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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