

# 2-Hepten-4-one, 2-hydroxy-6-methyl-

<b>Inchi:</b>	InChI=1S/C8H14O2/c1-6(2)4-8(10)5-7(3)9/h5-6,9H,4H2,1-3H3/b7-5-
<b>InchiKey:</b>	DUUWUNUXJISTIB-ALCCZGGFSA-N
<b>Formula:</b>	C8H14O2
<b>SMILES:</b>	CC(O)=CC(=O)CC(C)C
<b>Mol. weight [g/mol]:</b>	142.20
<b>CAS:</b>	81100-84-7

## Physical Properties

Property code	Value	Unit	Source
gf	-180.03	kJ/mol	Joback Method
hf	-371.11	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	56.48	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	2.063		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	532.09	K	Joback Method
tc	714.33	K	Joback Method
tf	256.63	K	Joback Method
vc	0.483	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.11	J/molxK	532.09	Joback Method
cpg	301.88	J/molxK	562.46	Joback Method
cpg	312.13	J/molxK	592.84	Joback Method
cpg	321.87	J/molxK	623.21	Joback Method
cpg	331.12	J/molxK	653.59	Joback Method
cpg	339.91	J/molxK	683.96	Joback Method
cpg	348.26	J/molxK	714.33	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C81100847&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C81100847&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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