

# 4-Methyl-3-hexen-2-one

<b>Inchi:</b>	InChI=1S/C7H12O/c1-4-6(2)5-7(3)8/h5H,4H2,1-3H3/b6-5+
<b>InchiKey:</b>	BGTFWRDJZNCBCV-AATRIKPKSA-N
<b>Formula:</b>	C7H12O
<b>SMILES:</b>	CCC(C)=CC(C)=O
<b>Mol. weight [g/mol]:</b>	112.17

## Physical Properties

Property code	Value	Unit	Source
gf	-49.19	kJ/mol	Joback Method
hf	-192.96	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	37.96	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.932		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3191.93	kPa	Joback Method
ripol	1240.00		NIST Webbook
ripol	1240.00		NIST Webbook
tb	417.47	K	Joback Method
tc	606.66	K	Joback Method
tf	199.54	K	Joback Method
vc	0.414	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.06	J/mol×K	417.47	Joback Method
cpg	211.30	J/mol×K	449.00	Joback Method
cpg	221.99	J/mol×K	480.53	Joback Method
cpg	232.15	J/mol×K	512.07	Joback Method
cpg	241.82	J/mol×K	543.60	Joback Method
cpg	251.01	J/mol×K	575.13	Joback Method
cpg	259.74	J/mol×K	606.66	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R340126&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R340126&amp;Units=SI</a>
<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>

# 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>hvp:</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>ripl:</b>	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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