

# 2-Methoxy-3-methyl-4-oxo-1-pentene

<b>Inchi:</b>	InChI=1S/C7H12O2/c1-5(6(2)8)7(3)9-4/h5H,3H2,1-2,4H3
<b>InchiKey:</b>	QQCBOBNMUPQOEEQ-UHFFFAOYSA-N
<b>Formula:</b>	C7H12O2
<b>SMILES:</b>	C=C(OC)C(C)C(C)=O
<b>Mol. weight [g/mol]:</b>	128.17
<b>CAS:</b>	82481-17-2

## Physical Properties

Property code	Value	Unit	Source
gf	-149.01	kJ/mol	Joback Method
hf	-322.25	kJ/mol	Joback Method
hfus	10.56	kJ/mol	Joback Method
hvap	39.35	kJ/mol	Joback Method
log10ws	-1.23		Crippen Method
logp	1.372		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	431.97	K	Joback Method
tc	619.68	K	Joback Method
tf	210.09	K	Joback Method
vc	0.427	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.88	J/molxK	431.97	Joback Method
cpg	233.85	J/molxK	463.25	Joback Method
cpg	244.40	J/molxK	494.54	Joback Method
cpg	254.52	J/molxK	525.82	Joback Method
cpg	264.23	J/molxK	557.11	Joback Method
cpg	273.52	J/molxK	588.39	Joback Method
cpg	282.41	J/molxK	619.68	Joback Method

# Sources

<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=C82481172&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82481172&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>

# 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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