

# 3-Chloro-2-methoxy-4-oxo-1-pentene

<b>Inchi:</b>	InChI=1S/C6H9ClO2/c1-4(8)6(7)5(2)9-3/h6H,2H2,1,3H3
<b>InchiKey:</b>	QMDIBXBGTZTPPR-UHFFFAOYSA-N
<b>Formula:</b>	C6H9ClO2
<b>SMILES:</b>	C=C(OC)C(Cl)C(C)=O
<b>Mol. weight [g/mol]:</b>	148.59
<b>CAS:</b>	82481-21-8

## Physical Properties

Property code	Value	Unit	Source
gf	-169.36	kJ/mol	Joback Method
hf	-317.35	kJ/mol	Joback Method
hfus	12.17	kJ/mol	Joback Method
hvap	41.51	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.343		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3341.24	kPa	Joback Method
tb	446.52	K	Joback Method
tc	642.86	K	Joback Method
tf	228.74	K	Joback Method
vc	0.420	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.96	J/molxK	446.52	Joback Method
cpg	218.31	J/molxK	479.24	Joback Method
cpg	227.25	J/molxK	511.97	Joback Method
cpg	235.79	J/molxK	544.69	Joback Method
cpg	243.95	J/molxK	577.41	Joback Method
cpg	251.71	J/molxK	610.13	Joback Method
cpg	259.10	J/molxK	642.86	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=C82481218&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82481218&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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