

# (E) Methyl 2-chloro-3-methoxy-2-butenate

<b>Inchi:</b>	InChI=1S/C6H9ClO3/c1-4(9-2)5(7)6(8)10-3/h1-3H3/b5-4+
<b>InchiKey:</b>	UCQQBIORXJIZBS-SNAWJCMRSA-N
<b>Formula:</b>	C6H9ClO3
<b>SMILES:</b>	COC(=O)C(Cl)=C(C)OC
<b>Mol. weight [g/mol]:</b>	164.59
<b>CAS:</b>	82481-24-1

## Physical Properties

Property code	Value	Unit	Source
gf	-288.09	kJ/mol	Joback Method
hf	-462.29	kJ/mol	Joback Method
hfus	17.05	kJ/mol	Joback Method
hvap	45.02	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.276		Crippen Method
mcvol	116.650	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	476.74	K	Joback Method
tc	676.44	K	Joback Method
tf	248.69	K	Joback Method
vc	0.445	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.15	J/molxK	476.74	Joback Method
cpg	238.42	J/molxK	510.02	Joback Method
cpg	247.33	J/molxK	543.31	Joback Method
cpg	255.86	J/molxK	576.59	Joback Method
cpg	264.02	J/molxK	609.87	Joback Method
cpg	271.81	J/molxK	643.15	Joback Method
cpg	279.23	J/molxK	676.44	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=C82481241&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82481241&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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