

# 2-Butenoic acid, 3-methoxy-2-methyl-, methyl ester, (Z)-

Inchi:	InChI=1S/C7H12O3/c1-5(6(2)9-3)7(8)10-4/h1-4H3/b6-5+
InchiKey:	BFLBTAHOAAXDNF-AATRIKPKSA-N
Formula:	C7H12O3
SMILES:	COC(=O)C(C)=C(C)OC
Mol. weight [g/mol]:	144.17
CAS:	82481-20-7

## Physical Properties

Property code	Value	Unit	Source
gf	-267.74	kJ/mol	Joback Method
hf	-467.19	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	42.86	kJ/mol	Joback Method
log10ws	-1.05		Crippen Method
logp	1.100		Crippen Method
mcvol	118.500	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	462.19	K	Joback Method
tc	653.57	K	Joback Method
tf	230.04	K	Joback Method
vc	0.452	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	244.97	J/molxK	462.19	Joback Method
cpg	255.87	J/molxK	494.09	Joback Method
cpg	266.36	J/molxK	525.98	Joback Method
cpg	276.45	J/molxK	557.88	Joback Method
cpg	286.14	J/molxK	589.78	Joback Method
cpg	295.43	J/molxK	621.67	Joback Method
cpg	304.32	J/molxK	653.57	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=C82481207&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C82481207&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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