

# 2-Methyl propyl 2-methyl 2-butenate

<b>Inchi:</b>	InChI=1S/C9H16O2/c1-5-8(4)9(10)11-6-7(2)3/h5,7H,6H2,1-4H3/b8-5+
<b>InchiKey:</b>	XDEGQMQRKHFPEBW-VMPITWQZSA-N
<b>Formula:</b>	C9H16O2
<b>SMILES:</b>	CC=C(C)C(=O)OCC(C)C
<b>Mol. weight [g/mol]:</b>	156.22

## Physical Properties

Property code	Value	Unit	Source
gf	-139.79	kJ/mol	Joback Method
hf	-371.74	kJ/mol	Joback Method
hfus	17.22	kJ/mol	Joback Method
hvap	44.43	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.152		Crippen Method
mvol	140.810	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
rinpol	1116.00		NIST Webbook
rinpol	1116.00		NIST Webbook
tb	485.21	K	Joback Method
tc	674.06	K	Joback Method
tf	229.31	K	Joback Method
vc	0.538	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.09	J/molxK	485.21	Joback Method
cpg	319.56	J/molxK	516.68	Joback Method
cpg	332.44	J/molxK	548.16	Joback Method
cpg	344.74	J/molxK	579.63	Joback Method
cpg	356.48	J/molxK	611.11	Joback Method
cpg	367.66	J/molxK	642.58	Joback Method
cpg	378.31	J/molxK	674.06	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=R515929&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R515929&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>h vap:</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>r in pol:</b>	Non-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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