

# 2-Butenoic acid, 2-methyl-, butyl ester, (Z)-

<b>Other names:</b>	Butyl angelate Angelic acid n-butyl ester butyl 2-methylcrotonate
<b>Inchi:</b>	InChI=1S/C9H16O2/c1-4-6-7-11-9(10)8(3)5-2/h5H,4,6-7H2,1-3H3/b8-5-
<b>InchiKey:</b>	RBGFLIOXJWFKKX-YVMONPNESA-N
<b>Formula:</b>	C9H16O2
<b>SMILES:</b>	CC=C(C)C(=O)OCCCC
<b>Mol. weight [g/mol]:</b>	156.22
<b>CAS:</b>	7785-64-0

## Physical Properties

Property code	Value	Unit	Source
gf	-137.35	kJ/mol	Joback Method
hf	-366.46	kJ/mol	Joback Method
hfus	20.74	kJ/mol	Joback Method
hvap	44.82	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.296		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1055.00		NIST Webbook
rinpol	1091.10		NIST Webbook
rinpol	1055.00		NIST Webbook
rinpol	1055.00		NIST Webbook
ripol	1417.00		NIST Webbook
tb	485.65	K	Joback Method
tc	670.48	K	Joback Method
tf	244.31	K	Joback Method
vc	0.544	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.90	J/mol×K	485.65	Joback Method

cpg	319.01	J/mol×K	516.46	Joback Method
cpg	331.57	J/mol×K	547.26	Joback Method
cpg	343.57	J/mol×K	578.07	Joback Method
cpg	355.04	J/mol×K	608.87	Joback Method
cpg	365.99	J/mol×K	639.68	Joback Method
cpg	376.43	J/mol×K	670.48	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=C7785640&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7785640&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>

## 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ripol:</b>	Non-polar retention indices
<b>ripol:</b>	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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