

# Methallyl angelate

<b>Other names:</b>	2-methylallyl 2-methylisocrotonate (Z)-2-Methylallyl 2-methylbut-2-enoate
<b>Inchi:</b>	InChI=1S/C9H14O2/c1-5-8(4)9(10)11-6-7(2)3/h5H,2,6H2,1,3-4H3/b8-5-
<b>InchiKey:</b>	PNRCWIZNCBKLHMH-YVMONPNESA-N
<b>Formula:</b>	C9H14O2
<b>SMILES:</b>	<chem>C=C(C)COC(=O)C(C)=CC</chem>
<b>Mol. weight [g/mol]:</b>	154.21
<b>CAS:</b>	61692-78-2

## Physical Properties

Property code	Value	Unit	Source
gf	-58.06	kJ/mol	Joback Method
hf	-250.82	kJ/mol	Joback Method
hfus	18.16	kJ/mol	Joback Method
hvap	44.23	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.072		Crippen Method
mvol	136.510	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinp	1068.80		NIST Webbook
tb	482.21	K	Joback Method
tc	674.32	K	Joback Method
tf	228.59	K	Joback Method
vc	0.526	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.32	J/molxK	482.21	Joback Method
cpg	301.01	J/molxK	514.23	Joback Method
cpg	313.11	J/molxK	546.25	Joback Method
cpg	324.62	J/molxK	578.26	Joback Method
cpg	335.58	J/molxK	610.28	Joback Method
cpg	346.00	J/molxK	642.30	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=C61692782&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61692782&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.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>rinpol:</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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