

# 2-Methylbutyl angelate

<b>Other names:</b>	2-methylbutyl 2-methylisocrotonate
<b>Inchi:</b>	InChI=1S/C10H18O2/c1-5-8(3)7-12-10(11)9(4)6-2/h6,8H,5,7H2,1-4H3/b9-6-
<b>InchiKey:</b>	DEJJNOHKWLTTKE-TWGQIWQCSA-N
<b>Formula:</b>	C10H18O2
<b>SMILES:</b>	CC=C(C)C(=O)OCC(C)CC
<b>Mol. weight [g/mol]:</b>	170.25
<b>CAS:</b>	61692-77-1

## Physical Properties

Property code	Value	Unit	Source
gf	-131.37	kJ/mol	Joback Method
hf	-392.38	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	46.66	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.542		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1158.50		NIST Webbook
rinpol	1134.00		NIST Webbook
ripol	1395.00		NIST Webbook
ripol	1395.00		NIST Webbook
tb	508.09	K	Joback Method
tc	694.82	K	Joback Method
tf	240.58	K	Joback Method
vc	0.595	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	350.82	J/mol×K	508.09	Joback Method
cpg	365.21	J/mol×K	539.21	Joback Method
cpg	378.95	J/mol×K	570.33	Joback Method
cpg	392.08	J/mol×K	601.46	Joback Method
cpg	404.60	J/mol×K	632.58	Joback Method
cpg	416.53	J/mol×K	663.70	Joback Method
cpg	427.88	J/mol×K	694.82	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=C61692771&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61692771&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>rinpol:</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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