

# Orcinyl angelate

<b>Inchi:</b>	InChI=1S/C12H14O3/c1-4-9(3)12(14)15-11-6-8(2)5-10(13)7-11/h4-7,13H,1-3H3/b9-4-
<b>InchiKey:</b>	AFRZSDNGGFCOLA-WTKPLQERSA-N
<b>Formula:</b>	C12H14O3
<b>SMILES:</b>	CC=C(C)C(=O)Oc1cc(C)cc(O)c1
<b>Mol. weight [g/mol]:</b>	206.24

## Physical Properties

Property code	Value	Unit	Source
gf	-163.93	kJ/mol	Joback Method
hf	-380.63	kJ/mol	Joback Method
hfus	27.95	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.572		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
ripol	2767.00		NIST Webbook
ripol	2767.00		NIST Webbook
tb	666.57	K	Joback Method
tc	895.59	K	Joback Method
tf	428.78	K	Joback Method
vc	0.571	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.33	J/molxK	666.57	Joback Method
cpg	437.20	J/molxK	704.74	Joback Method
cpg	449.27	J/molxK	742.91	Joback Method
cpg	460.61	J/molxK	781.08	Joback Method
cpg	471.32	J/molxK	819.25	Joback Method
cpg	481.48	J/molxK	857.42	Joback Method
cpg	491.17	J/molxK	895.59	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=R639382&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R639382&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.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>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>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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