

# Thymyl angelate

<b>Inchi:</b>	InChI=1S/C15H20O2/c1-6-12(5)15(16)17-14-9-11(4)7-8-13(14)10(2)3/h6-10H,1-5H3/b12
<b>InchiKey:</b>	UUEIVUJSJLKAAM-WUXMJOGZSA-N
<b>Formula:</b>	C15H20O2
<b>SMILES:</b>	CC=C(C)C(=O)Oc1cc(C)ccc1C(C)C
<b>Mol. weight [g/mol]:</b>	232.32
<b>CAS:</b>	101162-18-9

## Physical Properties

Property code	Value	Unit	Source
gf	3.88	kJ/mol	Joback Method
hf	-281.99	kJ/mol	Joback Method
hfus	26.03	kJ/mol	Joback Method
hvap	61.39	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.990		Crippen Method
mcvol	201.590	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinpol	1664.20		NIST Webbook
rinpol	1664.20		NIST Webbook
rinpol	1582.00		NIST Webbook
rinpol	1584.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2074.00		NIST Webbook
tb	659.13	K	Joback Method
tc	873.07	K	Joback Method
tf	348.39	K	Joback Method
vc	0.766	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	524.22	J/molxK	659.13	Joback Method
cpg	540.72	J/molxK	694.79	Joback Method
cpg	556.26	J/molxK	730.44	Joback Method

cpg	570.85	J/mol×K	766.10	Joback Method
cpg	584.54	J/mol×K	801.76	Joback Method
cpg	597.36	J/mol×K	837.42	Joback Method
cpg	609.35	J/mol×K	873.07	Joback Method

## Sources

<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>
<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=C101162189&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C101162189&amp;Units=SI</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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