

# Thymyl formate

<b>Inchi:</b>	InChI=1S/C11H14O2/c1-8(2)10-5-4-9(3)6-11(10)13-7-12/h4-8H,1-3H3
<b>InchiKey:</b>	IWAIRWGSZFYSES-UHFFFAOYSA-N
<b>Formula:</b>	C11H14O2
<b>SMILES:</b>	<chem>Cc1ccc(C(C)C)c(OC=O)c1</chem>
<b>Mol. weight [g/mol]:</b>	178.23

## Physical Properties

Property code	Value	Unit	Source
gf	-72.07	kJ/mol	Joback Method
hf	-279.86	kJ/mol	Joback Method
hfus	17.46	kJ/mol	Joback Method
hvap	52.42	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.654		Crippen Method
mcvol	149.530	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinsol	1262.00		NIST Webbook
tb	558.36	K	Joback Method
tc	769.26	K	Joback Method
tf	314.42	K	Joback Method
vc	0.573	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.05	J/molxK	558.36	Joback Method
cpg	360.93	J/molxK	593.51	Joback Method
cpg	374.09	J/molxK	628.66	Joback Method
cpg	386.55	J/molxK	663.81	Joback Method
cpg	398.32	J/molxK	698.96	Joback Method
cpg	409.40	J/molxK	734.11	Joback Method
cpg	419.80	J/molxK	769.26	Joback Method
dvisc	0.0018829	Paxs	314.42	Joback Method
dvisc	0.0010402	Paxs	355.08	Joback Method

dvisc	0.0006491	Paxs	395.73	Joback Method
dvisc	0.0004423	Paxs	436.39	Joback Method
dvisc	0.0003217	Paxs	477.05	Joback Method
dvisc	0.0002460	Paxs	517.70	Joback Method
dvisc	0.0001956	Paxs	558.36	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=R590846&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R590846&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>dvisc:</b>	Dynamic viscosity
<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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