

# thymyl valerate

<b>Inchi:</b>	InChI=1S/C15H22O2/c1-5-6-7-15(16)17-14-10-12(4)8-9-13(14)11(2)3/h8-11H,5-7H2,1-4
<b>InchiKey:</b>	RIJOKQDIPZLLFF-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O2
<b>SMILES:</b>	CCCCC(=O)Oc1cc(C)ccc1C(C)C
<b>Mol. weight [g/mol]:</b>	234.33

## Physical Properties

Property code	Value	Unit	Source
gf	-67.79	kJ/mol	Joback Method
hf	-389.42	kJ/mol	Joback Method
hfus	27.13	kJ/mol	Joback Method
hvap	61.35	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	4.214		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
ripol	1996.00		NIST Webbook
ripol	1996.00		NIST Webbook
tb	655.09	K	Joback Method
tc	857.92	K	Joback Method
tf	367.43	K	Joback Method
vc	0.785	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.23	J/molxK	655.09	Joback Method
cpg	621.07	J/molxK	824.11	Joback Method
cpg	607.86	J/molxK	790.31	Joback Method
cpg	593.79	J/molxK	756.50	Joback Method
cpg	578.84	J/molxK	722.70	Joback Method
cpg	562.99	J/molxK	688.89	Joback Method
cpg	633.44	J/molxK	857.92	Joback Method
dvisc	0.0001243	Paxs	655.09	Joback Method

dvisc	0.0001593	Paxs	607.15	Joback Method
dvisc	0.0002131	Paxs	559.20	Joback Method
dvisc	0.0003010	Paxs	511.26	Joback Method
dvisc	0.0004568	Paxs	463.32	Joback Method
dvisc	0.0007630	Paxs	415.37	Joback Method
dvisc	0.0014573	Paxs	367.43	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R522744&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R522744&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>
<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>

## 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>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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