

# Zingerone

<b>Inchi:</b>	InChI=1S/C11H14O3/c1-8(12)3-4-9-5-6-10(13)11(7-9)14-2/h5-7,13H,3-4H2,1-2H3
<b>InchiKey:</b>	OJYLAHXKWMRDGS-UHFFFAOYSA-N
<b>Formula:</b>	C11H14O3
<b>SMILES:</b>	<chem>COc1cc(CCC(C)=O)ccc1O</chem>
<b>Mol. weight [g/mol]:</b>	194.23

## Physical Properties

Property code	Value	Unit	Source
gf	-244.02	kJ/mol	Joback Method
hf	-467.42	kJ/mol	Joback Method
hfus	26.47	kJ/mol	Joback Method
hvap	65.19	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	1.922		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3217.33	kPa	Joback Method
rinpol	1529.00		NIST Webbook
tb	639.65	K	Joback Method
tc	859.98	K	Joback Method
tf	436.55	K	Joback Method
vc	0.533	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.49	J/molxK	639.65	Joback Method
cpg	410.14	J/molxK	676.37	Joback Method
cpg	422.03	J/molxK	713.09	Joback Method
cpg	433.22	J/molxK	749.81	Joback Method
cpg	443.76	J/molxK	786.54	Joback Method
cpg	453.72	J/molxK	823.26	Joback Method
cpg	463.15	J/molxK	859.98	Joback Method
dvisc	0.0005280	Paxs	436.55	Joback Method
dvisc	0.0002638	Paxs	470.40	Joback Method

dvisc	0.0001447	Paxs	504.25	Joback Method
dvisc	0.0000856	Paxs	538.10	Joback Method
dvisc	0.0000539	Paxs	571.95	Joback Method
dvisc	0.0000357	Paxs	605.80	Joback Method
dvisc	0.0000247	Paxs	639.65	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R613746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R613746&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>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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