

# Methyl zingerone

<b>Inchi:</b>	InChI=1S/C12H16O3/c1-9(13)4-5-10-6-7-11(14-2)12(8-10)15-3/h6-8H,4-5H2,1-3H3
<b>InchiKey:</b>	RVTJUTXCUYSHAZ-UHFFFAOYSA-N
<b>Formula:</b>	C12H16O3
<b>SMILES:</b>	<chem>COc1ccc(CCC(C)=O)cc1OC</chem>
<b>Mol. weight [g/mol]:</b>	208.25
<b>CAS:</b>	6302-60-9

## Physical Properties

Property code	Value	Unit	Source
gf	-195.61	kJ/mol	Joback Method
hf	-454.44	kJ/mol	Joback Method
hfus	24.07	kJ/mol	Joback Method
hvap	57.47	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.225		Crippen Method
mcvol	169.490	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1696.10		NIST Webbook
rinpol	1696.10		NIST Webbook
ripol	2640.00		NIST Webbook
ripol	2640.00		NIST Webbook
tb	609.31	K	Joback Method
tc	815.15	K	Joback Method
tf	370.85	K	Joback Method
vc	0.641	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.81	J/molxK	609.31	Joback Method
cpg	433.24	J/molxK	643.62	Joback Method
cpg	446.94	J/molxK	677.92	Joback Method
cpg	459.92	J/molxK	712.23	Joback Method

cpg	472.17	J/molxK	746.54	Joback Method
cpg	483.69	J/molxK	780.85	Joback Method
cpg	494.48	J/molxK	815.15	Joback Method
dvisc	0.0010176	Paxs	370.85	Joback Method
dvisc	0.0006260	Paxs	410.59	Joback Method
dvisc	0.0004195	Paxs	450.34	Joback Method
dvisc	0.0003000	Paxs	490.08	Joback Method
dvisc	0.0002256	Paxs	529.82	Joback Method
dvisc	0.0001766	Paxs	569.57	Joback Method
dvisc	0.0001427	Paxs	609.31	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6302609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6302609&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>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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