

# Phenol, 2,6-dimethoxy-4-(5,5-dimethyl-2-oxazolin-2-yl)-

Inchi:	InChI=1S/C13H17NO4/c1-13(2)7-14-12(18-13)8-5-9(16-3)11(15)10(6-8)17-4/h5-6,15H,7
InchiKey:	YNKGMQRKAGQBMD-UHFFFAOYSA-N
Formula:	C13H17NO4
SMILES:	COc1cc(C2=NCC(C)(C)O2)cc(OC)c1O
Mol. weight [g/mol]:	251.28
CAS:	116595-28-9

## Physical Properties

Property code	Value	Unit	Source
gf	-130.84	kJ/mol	Joback Method
hf	-478.81	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	76.75	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.965		Crippen Method
mcvol	188.570	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	759.25	K	Joback Method
tc	1005.29	K	Joback Method
tf	590.10	K	Joback Method
vc	0.652	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	565.58	J/molxK	759.25	Joback Method
cpg	581.75	J/molxK	800.26	Joback Method
cpg	597.34	J/molxK	841.26	Joback Method
cpg	612.52	J/molxK	882.27	Joback Method
cpg	627.45	J/molxK	923.28	Joback Method
cpg	642.29	J/molxK	964.29	Joback Method
cpg	657.20	J/molxK	1005.29	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=C116595289&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595289&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>

# 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>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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