

# Ylangenal

<b>Inchi:</b>	InChI=1S/C15H22O/c1-9(2)11-6-7-15(3)12-5-4-10(8-16)14(15)13(11)12/h4,8-9,11-14H,5
<b>InchiKey:</b>	IDQMMWVVRDXRNI-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC(C)C1CCC2(C)C3CC=C(C=O)C2C13
<b>Mol. weight [g/mol]:</b>	218.33
<b>CAS:</b>	41610-68-8

## Physical Properties

Property code	Value	Unit	Source
gf	143.03	kJ/mol	Joback Method
hf	-210.68	kJ/mol	Joback Method
hfus	22.35	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.450		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1674.60		NIST Webbook
rinpol	1674.60		NIST Webbook
tb	610.35	K	Joback Method
tc	826.83	K	Joback Method
tf	364.81	K	Joback Method
vc	0.732	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.68	J/mol×K	610.35	Joback Method
cpg	551.80	J/mol×K	646.43	Joback Method
cpg	570.67	J/mol×K	682.51	Joback Method
cpg	588.49	J/mol×K	718.59	Joback Method
cpg	605.44	J/mol×K	754.67	Joback Method
cpg	621.69	J/mol×K	790.75	Joback Method
cpg	637.44	J/mol×K	826.83	Joback Method

# Sources

<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=C41610688&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41610688&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>

# 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>h vap:</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>r in pol:</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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