

# Ylangene

<b>Other names:</b>	Tricyclo[4.4.0.0(2,7)]dec-3-ene, 8-isopropyl-1,3-dimethyl-, (1S,2R,6R,7R,8S)-(+)- (1S,2R,6R,7R,8S)-8-Isopropyl-1,3-dimethyltricyclo[4.4.0.0(2,7)]dec-3-ene Tricyclo[4.4.0.0(2,7)]dec-3-ene, 1,3-dimethyl-8-(1-methylethyl)-, stereoisomer «alpha»-Ylangene (+)-Ylangene d-Ylangene «alpha»-Yalangene (+)-«alpha»-Ylangene
<b>Inchi:</b>	InChI=1S/C15H24/c1-9(2)11-7-8-15(4)12-6-5-10(3)14(15)13(11)12/h5,9,11-14H,6-8H2,1
<b>InchiKey:</b>	VLXDPFLIRFYIME-XTLGRWLVSA-N
<b>Formula:</b>	C15H24
<b>SMILES:</b>	CC1=CCC2C3C(C(C)C)CCC2(C)C13
<b>Mol. weight [g/mol]:</b>	204.35
<b>CAS:</b>	14912-44-8

## Physical Properties

Property code	Value	Unit	Source
gf	242.55	kJ/mol	Joback Method
hf	-125.10	kJ/mol	Joback Method
hfus	20.07	kJ/mol	Joback Method
hvap	47.69	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.271		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	1354.00		NIST Webbook
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ripol	1491.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	561.69	K	Joback Method
tc	775.53	K	Joback Method
tf	322.81	K	Joback Method
vc	0.715	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.35	J/molxK	561.69	Joback Method
cpg	525.87	J/molxK	597.33	Joback Method
cpg	546.93	J/molxK	632.97	Joback Method
cpg	566.70	J/molxK	668.61	Joback Method
cpg	585.36	J/molxK	704.25	Joback Method
cpg	603.09	J/molxK	739.89	Joback Method
cpg	620.07	J/molxK	775.53	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C14912448&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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>rinpola:</b>	Non-polar retention indices
<b>ripola:</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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