

# Calamenol 2

<b>Inchi:</b>	InChI=1S/C15H22O/c1-9(2)12-7-5-10(3)13-8-6-11(4)15(16)14(12)13/h6,8-10,12,16H,5,7
<b>InchiKey:</b>	YXYMGKMWKSMRAB-UHFFFAOYSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	Cc1ccc2c(c1O)C(C(C)C)CCC2C
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	52.45	kJ/mol	Joback Method
hf	-275.63	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.338		Crippen Method
mvol	193.460	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	1665.00		NIST Webbook
tb	665.76	K	Joback Method
tc	893.47	K	Joback Method
tf	417.17	K	Joback Method
vc	0.675	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.17	J/molxK	665.76	Joback Method
cpg	629.78	J/molxK	855.52	Joback Method
cpg	615.14	J/molxK	817.56	Joback Method
cpg	599.66	J/molxK	779.61	Joback Method
cpg	583.24	J/molxK	741.66	Joback Method
cpg	565.78	J/molxK	703.71	Joback Method
cpg	643.69	J/molxK	893.47	Joback Method
dvisc	0.0000379	Paxs	665.76	Joback Method
dvisc	0.0000546	Paxs	624.33	Joback Method

dvisc	0.0000827	Paxs	582.90	Joback Method
dvisc	0.0001337	Paxs	541.47	Joback Method
dvisc	0.0002338	Paxs	500.03	Joback Method
dvisc	0.0004524	Paxs	458.60	Joback Method
dvisc	0.0009983	Paxs	417.17	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R517698&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R517698&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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