

# Calamenene oxide

**Inchi:** InChI=1S/C14H18O/c1-13(2)11-8-9-14(3,15-13)12-7-5-4-6-10(11)12/h4-7,11H,8-9H2,1-3H  
**InchiKey:** UPULKYWOGKVXOB-UHFFFAOYSA-N  
**Formula:** C14H18O  
**SMILES:** CC12CCC(c3ccccc31)C(C)(C)O2  
**Mol. weight [g/mol]:** 202.29

## Physical Properties

Property code	Value	Unit	Source
gf	186.47	kJ/mol	Joback Method
hf	-83.49	kJ/mol	Joback Method
hfus	18.39	kJ/mol	Joback Method
hvap	51.42	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.588		Crippen Method
mcvol	168.510	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1481.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1481.00		NIST Webbook
tb	587.62	K	Joback Method
tc	828.85	K	Joback Method
tf	392.49	K	Joback Method
vc	0.641	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.95	J/molxK	587.62	Joback Method
cpg	464.65	J/molxK	627.82	Joback Method
cpg	482.01	J/molxK	668.03	Joback Method
cpg	498.38	J/molxK	708.23	Joback Method
cpg	514.11	J/molxK	748.44	Joback Method
cpg	529.56	J/molxK	788.64	Joback Method
cpg	545.09	J/molxK	828.85	Joback Method

# Sources

<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=R202014&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R202014&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>rinpola:</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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