

# 1,11-Oxidocalamenene

<b>Inchi:</b>	InChI=1S/C15H20O/c1-10-5-6-13-11(9-10)12-7-8-15(13,4)16-14(12,2)3/h5-6,9,12H,7-8H
<b>InchiKey:</b>	RWNMGACJGXHHHN-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O
<b>SMILES:</b>	<chem>Cc1ccc2c(c1)C1CCC2(C)OC1(C)C</chem>
<b>Mol. weight [g/mol]:</b>	216.32

## Physical Properties

Property code	Value	Unit	Source
gf	185.26	kJ/mol	Joback Method
hf	-115.60	kJ/mol	Joback Method
hfus	20.59	kJ/mol	Joback Method
hvap	54.31	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.896		Crippen Method
mcvol	182.600	ml/mol	McGowan Method
pc	2381.86	kPa	Joback Method
ripol	1490.00		NIST Webbook
ripol	1898.00		NIST Webbook
ripol	1898.00		NIST Webbook
tb	615.48	K	Joback Method
tc	852.68	K	Joback Method
tf	416.28	K	Joback Method
vc	0.698	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	496.08	J/mol×K	615.48	Joback Method
cpg	514.95	J/mol×K	655.01	Joback Method
cpg	532.70	J/mol×K	694.55	Joback Method
cpg	549.68	J/mol×K	734.08	Joback Method
cpg	566.21	J/mol×K	773.61	Joback Method
cpg	582.64	J/mol×K	813.15	Joback Method
cpg	599.28	J/mol×K	852.68	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R292636&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R292636&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>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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