

# 14-Oxo-calamene

<b>Inchi:</b>	InChI=1S/C15H20O/c1-10(2)13-6-4-11(3)14-7-5-12(9-16)8-15(13)14/h4,6,9-10,12H,5,7-8
<b>InchiKey:</b>	LYDWFRQFTHOVPU-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O
<b>SMILES:</b>	<chem>Cc1ccc(C(C)C)c2c1CCC(C=O)C2</chem>
<b>Mol. weight [g/mol]:</b>	216.32

## Physical Properties

Property code	Value	Unit	Source
gf	105.63	kJ/mol	Joback Method
hf	-175.03	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.422		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
ripol	2470.00		NIST Webbook
tb	643.45	K	Joback Method
tc	865.02	K	Joback Method
tf	364.21	K	Joback Method
vc	0.728	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.92	J/molxK	643.45	Joback Method
cpg	585.16	J/molxK	828.09	Joback Method
cpg	571.35	J/molxK	791.17	Joback Method
cpg	556.58	J/molxK	754.24	Joback Method
cpg	540.78	J/molxK	717.31	Joback Method
cpg	523.92	J/molxK	680.38	Joback Method
cpg	598.06	J/molxK	865.02	Joback Method
dvisc	0.0003260	Paxs	643.45	Joback Method
dvisc	0.0003924	Paxs	596.91	Joback Method

dvisc	0.0004874	Paxs	550.37	Joback Method
dvisc	0.0006301	Paxs	503.83	Joback Method
dvisc	0.0008584	Paxs	457.29	Joback Method
dvisc	0.0012543	Paxs	410.75	Joback Method
dvisc	0.0020191	Paxs	364.21	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R420103&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R420103&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>ripol:</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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