

# Lophenone

<b>Inchi:</b>	InChI=1S/C28H46O/c1-18(2)8-7-9-19(3)22-12-13-24-21-10-11-23-20(4)26(29)15-17-28(2)
<b>InchiKey:</b>	OWKGVXPXWOHLTSL-LAIDNRQRSA-N
<b>Formula:</b>	C28H46O
<b>SMILES:</b>	CC(C)CCCC(C)C1CCC2C3=CCC4C(C)C(=O)CCC4(C)C3CCC21C
<b>Mol. weight [g/mol]:</b>	398.66

## Physical Properties

Property code	Value	Unit	Source
gf	226.13	kJ/mol	Joback Method
hf	-493.34	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	79.63	kJ/mol	Joback Method
log10ws	-8.08		Crippen Method
logp	7.843		Crippen Method
mvol	359.210	ml/mol	McGowan Method
pc	977.78	kPa	Joback Method
rinpol	3210.00		NIST Webbook
rinpol	3210.00		NIST Webbook
tb	945.90	K	Joback Method
tc	1178.17	K	Joback Method
tf	546.06	K	Joback Method
vc	1.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1347.42	J/molxK	945.90	Joback Method
cpg	1379.45	J/molxK	984.61	Joback Method
cpg	1411.68	J/molxK	1023.32	Joback Method
cpg	1444.44	J/molxK	1062.03	Joback Method
cpg	1478.05	J/molxK	1100.74	Joback Method
cpg	1512.85	J/molxK	1139.45	Joback Method
cpg	1549.16	J/molxK	1178.17	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R596879&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R596879&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>hvpap:</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>rinppl:</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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