

# Lophenol acetate

<b>Inchi:</b>	InChI=1S/C30H50O2/c1-19(2)9-8-10-20(3)24-13-14-26-23-11-12-25-21(4)28(32-22(5)31
<b>InchiKey:</b>	SQJKDEQVXPFQGL-APFUBLHXSA-N
<b>Formula:</b>	C30H50O2
<b>SMILES:</b>	CC(=O)OC1CCC2(C)C3CCC4(C)C(CCC4C(C)CCCC(C)C)C3=CCC2C1C
<b>Mol. weight [g/mol]:</b>	442.72

## Physical Properties

Property code	Value	Unit	Source
gf	123.93	kJ/mol	Joback Method
hf	-662.06	kJ/mol	Joback Method
hfus	43.76	kJ/mol	Joback Method
hvap	88.68	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	8.206		Crippen Method
mcvol	393.260	ml/mol	McGowan Method
pc	858.98	kPa	Joback Method
rinpol	3275.00		NIST Webbook
tb	995.46	K	Joback Method
tc	1225.14	K	Joback Method
tf	568.30	K	Joback Method
vc	1.494	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1506.50	J/mol×K	995.46	Joback Method
cpg	1539.96	J/mol×K	1033.74	Joback Method
cpg	1573.93	J/mol×K	1072.02	Joback Method
cpg	1608.76	J/mol×K	1110.30	Joback Method
cpg	1644.77	J/mol×K	1148.58	Joback Method
cpg	1682.29	J/mol×K	1186.86	Joback Method
cpg	1721.67	J/mol×K	1225.14	Joback Method

# Sources

<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=R111334&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R111334&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>

# 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>h vap:</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>m cvol:</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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