

# 4-geraniloxy-«gamma»-valeroladone

<b>Inchi:</b>	InChI=1S/C15H24O3/c1-11(2)6-5-7-12(3)8-9-17-14-10-15(16)18-13(14)4/h6,8,13-14H,5,
<b>InchiKey:</b>	LHKUAUJLJDLCKN-XYOKQWHBSA-N
<b>Formula:</b>	C15H24O3
<b>SMILES:</b>	CC(C)=CCCC(C)=CCOC1CC(=O)OC1C
<b>Mol. weight [g/mol]:</b>	252.35

## Physical Properties

Property code	Value	Unit	Source
gf	-66.11	kJ/mol	Joback Method
hf	-499.85	kJ/mol	Joback Method
hfus	36.07	kJ/mol	Joback Method
hvap	60.17	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.400		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
ripol	2572.00		NIST Webbook
tb	678.48	K	Joback Method
tc	888.60	K	Joback Method
tf	344.41	K	Joback Method
vc	0.824	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	619.07	J/mol×K	678.48	Joback Method
cpg	638.55	J/mol×K	713.50	Joback Method
cpg	656.93	J/mol×K	748.52	Joback Method
cpg	674.21	J/mol×K	783.54	Joback Method
cpg	690.45	J/mol×K	818.56	Joback Method
cpg	705.64	J/mol×K	853.58	Joback Method
cpg	719.84	J/mol×K	888.60	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=R321432&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R321432&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>
<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>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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