

# 4-Epipallensin

<b>Inchi:</b>	InChI=1S/C15H20O4/c1-8-9-4-6-14(2)10(16)5-7-15(3,18)12(14)11(9)19-13(8)17/h5,7-9,1
<b>InchiKey:</b>	NGPDZEACIWDCCKX-UHFFFAOYSA-N
<b>Formula:</b>	C15H20O4
<b>SMILES:</b>	CC1C(=O)OC2C1CCC1(C)C(=O)C=CC(C)(O)C21
<b>Mol. weight [g/mol]:</b>	264.32
<b>CAS:</b>	1275525-60-4

## Physical Properties

Property code	Value	Unit	Source
gf	-263.00	kJ/mol	Joback Method
hf	-691.56	kJ/mol	Joback Method
hfus	23.54	kJ/mol	Joback Method
hvap	76.16	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.470		Crippen Method
mvol	200.210	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	2159.70		NIST Webbook
rinpol	2159.70		NIST Webbook
tb	820.30	K	Joback Method
tc	1059.26	K	Joback Method
tf	558.22	K	Joback Method
vc	0.748	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.56	J/mol×K	820.30	Joback Method
cpg	707.76	J/mol×K	860.13	Joback Method
cpg	727.84	J/mol×K	899.95	Joback Method
cpg	748.03	J/mol×K	939.78	Joback Method
cpg	768.57	J/mol×K	979.60	Joback Method
cpg	789.71	J/mol×K	1019.43	Joback Method
cpg	811.69	J/mol×K	1059.26	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1275525604&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1275525604&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpolar:</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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