

# Germacranolide callitris

<b>Inchi:</b>	InChI=1S/C15H22O2/c1-10-5-4-6-11(2)9-14-13(8-7-10)12(3)15(16)17-14/h6-7,12-14H,4-
<b>InchiKey:</b>	QJRFOUJEGHRZIU-NXAIOARDSA-N
<b>Formula:</b>	C15H22O2
<b>SMILES:</b>	CC1=CCC2C(CC(C)=CCC1)OC(=O)C2C
<b>Mol. weight [g/mol]:</b>	234.33
<b>CAS:</b>	57759-35-0

## Physical Properties

Property code	Value	Unit	Source
gf	-63.54	kJ/mol	Joback Method
hf	-447.87	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.631		Crippen Method
mvol	199.330	ml/mol	McGowan Method
pc	2088.84	kPa	Joback Method
rinpol	1972.80		NIST Webbook
rinpol	1972.80		NIST Webbook
tb	684.35	K	Joback Method
tc	927.07	K	Joback Method
tf	387.16	K	Joback Method
vc	0.733	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.87	J/mol×K	684.35	Joback Method
cpg	609.93	J/mol×K	724.80	Joback Method
cpg	631.32	J/mol×K	765.26	Joback Method
cpg	651.02	J/mol×K	805.71	Joback Method
cpg	669.03	J/mol×K	846.17	Joback Method
cpg	685.32	J/mol×K	886.62	Joback Method
cpg	699.89	J/mol×K	927.07	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C57759350&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57759350&amp;Units=SI</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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