

# (R)-(+)-Citronellic acid, 4,4-dimethyloxazoline (dmox) derivative

Inchi:	InChI=1S/C14H25NO/c1-11(2)7-6-8-12(3)9-13-15-14(4,5)10-16-13/h7,12H,6,8-10H2,1-5
InchiKey:	MEMKUNKVVADDCW-UHFFFAOYSA-N
Formula:	C14H25NO
SMILES:	CC(C)=CCCC(C)CC1=NC(C)(C)CO1
Mol. weight [g/mol]:	223.35

## Physical Properties

Property code	Value	Unit	Source
gf	218.28	kJ/mol	Joback Method
hf	-169.14	kJ/mol	Joback Method
hfus	28.97	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	3.966		Crippen Method
mcvol	204.510	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
rinpol	1450.80		NIST Webbook
rinpol	1450.80		NIST Webbook
tb	623.63	K	Joback Method
tc	836.81	K	Joback Method
tf	359.69	K	Joback Method
vc	0.789	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.32	J/mol×K	623.63	Joback Method
cpg	586.37	J/mol×K	659.16	Joback Method
cpg	605.34	J/mol×K	694.69	Joback Method
cpg	623.36	J/mol×K	730.22	Joback Method
cpg	640.55	J/mol×K	765.75	Joback Method
cpg	657.02	J/mol×K	801.28	Joback Method
cpg	672.91	J/mol×K	836.81	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U333589&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U333589&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>

# 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>rinpola:</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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