

# Citronellyl isocrotonate

<b>Inchi:</b>	InChI=1S/C14H24O2/c1-5-7-14(15)16-11-10-13(4)9-6-8-12(2)3/h5,7-8,13H,6,9-11H2,1-4
<b>InchiKey:</b>	MYGZJMACIRJNPL-ALCCZGGFSA-N
<b>Formula:</b>	C14H24O2
<b>SMILES:</b>	CC=CC(=O)OCCC(C)CCC=C(C)C
<b>Mol. weight [g/mol]:</b>	224.34

## Physical Properties

Property code	Value	Unit	Source
gf	-17.47	kJ/mol	Joback Method
hf	-357.72	kJ/mol	Joback Method
hfus	30.37	kJ/mol	Joback Method
hvap	55.52	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.878		Crippen Method
mcvol	206.960	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
ripol	1833.00		NIST Webbook
ripol	1833.00		NIST Webbook
tb	603.77	K	Joback Method
tc	789.85	K	Joback Method
tf	280.58	K	Joback Method
vc	0.798	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.76	J/molxK	603.77	Joback Method
cpg	544.41	J/molxK	634.78	Joback Method
cpg	560.24	J/molxK	665.80	Joback Method
cpg	575.29	J/molxK	696.81	Joback Method
cpg	589.60	J/molxK	727.82	Joback Method
cpg	603.19	J/molxK	758.84	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=R409577&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R409577&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>

## 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>rinpol:</b>	Non-polar retention indices
<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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