

# Citryl acetate

<b>Inchi:</b>	InChI=1S/C13H20O2/c1-10-4-6-13(7-5-10)11(2)8-9-15-12(3)14/h4,8,13H,5-7,9H2,1-3H3
<b>InchiKey:</b>	VRZUSHXWKUAXEH-FLIBITNWSA-N
<b>Formula:</b>	C13H20O2
<b>SMILES:</b>	CC(=O)OCC=C(C)C1CC=C(C)CC1
<b>Mol. weight [g/mol]:</b>	208.30

## Physical Properties

Property code	Value	Unit	Source
gf	-58.89	kJ/mol	Joback Method
hf	-348.39	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	55.11	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.242		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
pc	2189.73	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	600.86	K	Joback Method
tc	812.01	K	Joback Method
tf	310.05	K	Joback Method
vc	0.688	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.15	J/mol×K	600.86	Joback Method
cpg	484.32	J/mol×K	636.05	Joback Method
cpg	501.46	J/mol×K	671.24	Joback Method
cpg	517.60	J/mol×K	706.43	Joback Method
cpg	532.78	J/mol×K	741.63	Joback Method
cpg	547.01	J/mol×K	776.82	Joback Method
cpg	560.33	J/mol×K	812.01	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=R331489&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R331489&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>
<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>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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