

# Citrol

<b>Inchi:</b>	InChI=1S/C11H18O/c1-9-3-5-11(6-4-9)10(2)7-8-12/h3,7,11-12H,4-6,8H2,1-2H3/b10-7-
<b>InchiKey:</b>	BMSVWDJXCKMWSV-YFHOEESVSA-N
<b>Formula:</b>	C11H18O
<b>SMILES:</b>	CC1=CCC(C(C)=CCO)CC1
<b>Mol. weight [g/mol]:</b>	166.26

## Physical Properties

Property code	Value	Unit	Source
gf	21.37	kJ/mol	Joback Method
hf	-214.54	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	58.18	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.671		Crippen Method
mcvol	152.260	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
rinqol	1255.00		NIST Webbook
tb	570.99	K	Joback Method
tc	768.68	K	Joback Method
tf	276.17	K	Joback Method
vc	0.571	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.68	J/mol×K	570.99	Joback Method
cpg	395.15	J/mol×K	603.94	Joback Method
cpg	409.77	J/mol×K	636.89	Joback Method
cpg	423.59	J/mol×K	669.83	Joback Method
cpg	436.63	J/mol×K	702.78	Joback Method
cpg	448.94	J/mol×K	735.73	Joback Method
cpg	460.55	J/mol×K	768.68	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=R567950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R567950&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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