

# Photocitral A

<b>Inchi:</b>	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)10(9)6-11/h6,8-10H,1,4-5H2,2-3H3/t8-,9-,10-/m0/s
<b>InchiKey:</b>	JCDLXWAYWSJVTP-GUBZILKMSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	C=C(C)C1CCC(C)C1C=O
<b>Mol. weight [g/mol]:</b>	152.23

## Physical Properties

Property code	Value	Unit	Source
gf	34.22	kJ/mol	Joback Method
hf	-199.87	kJ/mol	Joback Method
hfus	17.43	kJ/mol	Joback Method
hvap	43.62	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.424		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2648.83	kPa	Joback Method
rinpol	1123.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1118.00		NIST Webbook
rinpol	1125.00		NIST Webbook
rinpol	1123.00		NIST Webbook
rinpol	1125.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1515.00		NIST Webbook
tb	479.36	K	Joback Method
tc	681.52	K	Joback Method
tf	231.16	K	Joback Method
vc	0.533	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.37	J/molxK	479.36	Joback Method
cpg	328.76	J/molxK	513.05	Joback Method

cpg	345.26	J/mol×K	546.75	Joback Method
cpg	360.90	J/mol×K	580.44	Joback Method
cpg	375.71	J/mol×K	614.13	Joback Method
cpg	389.72	J/mol×K	647.82	Joback Method
cpg	402.93	J/mol×K	681.52	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.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=U292850&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292850&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>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>ripola:</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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