

# epiphotocitral 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
<b>InchiKey:</b>	JCDLXWAYWSJVTP-UHFFFAOYSA-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	1113.00		NIST Webbook
rinpol	1113.00		NIST Webbook
ripol	1492.00		NIST Webbook
tb	479.36	K	Joback Method
tc	681.52	K	Joback Method
tf	231.16	K	Joback Method
vc	0.533	m3/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/molxK	546.75	Joback Method
cpg	360.90	J/molxK	580.44	Joback Method
cpg	375.71	J/molxK	614.13	Joback Method
cpg	389.72	J/molxK	647.82	Joback Method
cpg	402.93	J/molxK	681.52	Joback Method

# Sources

<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=U365938&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U365938&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>

# 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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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