

# photocitral B

<b>Inchi:</b>	InChI=1S/C10H16O/c1-9(2)7-4-5-10(9,3)8(7)6-11/h6-8H,4-5H2,1-3H3
<b>InchiKey:</b>	AGTSNXAZDKAPHU-UHFFFAOYSA-N
<b>Formula:</b>	C10H16O
<b>SMILES:</b>	CC1(C)C2CCC1(C)C2C=O
<b>Mol. weight [g/mol]:</b>	152.23
<b>CAS:</b>	6040-45-5

## Physical Properties

Property code	Value	Unit	Source
gf	28.90	kJ/mol	Joback Method
hf	-199.91	kJ/mol	Joback Method
hfus	9.76	kJ/mol	Joback Method
hvap	41.48	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.258		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1078.00		NIST Webbook
ripol	1434.00		NIST Webbook
tb	481.48	K	Joback Method
tc	693.12	K	Joback Method
tf	319.66	K	Joback Method
vc	0.520	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	316.35	J/molxK	481.48	Joback Method
cpg	333.54	J/molxK	516.75	Joback Method
cpg	349.24	J/molxK	552.03	Joback Method
cpg	363.66	J/molxK	587.30	Joback Method
cpg	377.04	J/molxK	622.57	Joback Method

cpg	389.59	J/mol×K	657.85	Joback Method
cpg	401.54	J/mol×K	693.12	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=C6040455&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6040455&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>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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