

# «alpha»-Campholenyl acetate

<b>Inchi:</b>	InChI=1S/C12H20O2/c1-9-5-6-11(12(9,3)4)7-8-14-10(2)13/h5,11H,6-8H2,1-4H3
<b>InchiKey:</b>	HBRWKAJTMKFEQR-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	CC(=O)OCCC1CC=C(C)C1(C)C
<b>Mol. weight [g/mol]:</b>	196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-140.08	kJ/mol	Joback Method
hf	-434.12	kJ/mol	Joback Method
hfus	19.16	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.932		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1316.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1316.00		NIST Webbook
rinpol	1317.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1681.00		NIST Webbook
tb	565.24	K	Joback Method
tc	768.19	K	Joback Method
tf	341.00	K	Joback Method
vc	0.655	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.72	J/molxK	565.24	Joback Method
cpg	450.77	J/molxK	599.06	Joback Method
cpg	466.95	J/molxK	632.89	Joback Method
cpg	482.34	J/molxK	666.71	Joback Method

cpg	497.01	J/mol×K	700.54	Joback Method
cpg	511.05	J/mol×K	734.36	Joback Method
cpg	524.55	J/mol×K	768.19	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=R204629&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R204629&amp;Units=SI</a>
<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>

## 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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