

# «alpha»-Cyclogeraniol, acetate

<b>Inchi:</b>	InChI=1S/C12H20O2/c1-9-6-5-7-12(3,4)11(9)8-14-10(2)13/h5-8H2,1-4H3
<b>InchiKey:</b>	FTIUTTJEFHWCSA-UHFFFAOYSA-N
<b>Formula:</b>	C12H20O2
<b>SMILES:</b>	CC(=O)OCC1=C(C)CCCC1(C)C
<b>Mol. weight [g/mol]:</b>	196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-154.10	kJ/mol	Joback Method
hf	-431.41	kJ/mol	Joback Method
hfus	15.60	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.076		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinsol	1471.00		NIST Webbook
tb	579.16	K	Joback Method
tc	790.19	K	Joback Method
tf	354.24	K	Joback Method
vc	0.648	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.72	J/mol×K	579.16	Joback Method
cpg	450.99	J/mol×K	614.33	Joback Method
cpg	467.37	J/mol×K	649.50	Joback Method
cpg	482.95	J/mol×K	684.67	Joback Method
cpg	497.82	J/mol×K	719.85	Joback Method
cpg	512.06	J/mol×K	755.02	Joback Method
cpg	525.76	J/mol×K	790.19	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=R129736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R129736&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>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>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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