

# (E)-12-Norcaryophyll-5-en-2-one

<b>Inchi:</b>	InChI=1S/C14H22O/c1-10-5-4-6-13(15)11-9-14(2,3)12(11)8-7-10/h5,11-12H,4,6-9H2,1-3
<b>InchiKey:</b>	MBZBBVTYLUNZPJ-BJMVG YQFSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC1=CCCC(=O)C2CC(C)(C)C2CC1
<b>Mol. weight [g/mol]:</b>	206.32

## Physical Properties

Property code	Value	Unit	Source
gf	12.54	kJ/mol	Joback Method
hf	-313.98	kJ/mol	Joback Method
hfus	12.90	kJ/mol	Joback Method
hvap	51.19	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.738		Crippen Method
mcvol	183.670	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1984.00		NIST Webbook
tb	622.08	K	Joback Method
tc	863.67	K	Joback Method
tf	366.98	K	Joback Method
vc	0.683	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.19	J/mol×K	622.08	Joback Method
cpg	534.48	J/mol×K	662.35	Joback Method
cpg	556.40	J/mol×K	702.61	Joback Method
cpg	577.08	J/mol×K	742.88	Joback Method
cpg	596.66	J/mol×K	783.14	Joback Method
cpg	615.26	J/mol×K	823.41	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=R241559&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R241559&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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