

# Isolongifolen-9-one

<b>Inchi:</b>	InChI=1S/C15H22O/c1-13(2)7-5-6-12-14(3,4)10-8-15(12,13)9-11(10)16/h6,10H,5,7-9H2,
<b>InchiKey:</b>	ZNAKKZNXJRNCAC-BONVTFDSA-N
<b>Formula:</b>	C15H22O
<b>SMILES:</b>	CC1(C)C2=CCCC(C)(C)C23CC(=O)C1C3
<b>Mol. weight [g/mol]:</b>	218.33

## Physical Properties

Property code	Value	Unit	Source
gf	107.03	kJ/mol	Joback Method
hf	-212.86	kJ/mol	Joback Method
hfus	7.33	kJ/mol	Joback Method
hvap	50.51	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpola	1663.90		NIST Webbook
rinpola	1663.90		NIST Webbook
rinpola	1645.00		NIST Webbook
rinpola	1627.90		NIST Webbook
tb	639.37	K	Joback Method
tc	887.45	K	Joback Method
tf	454.55	K	Joback Method
vc	0.717	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.19	J/molxK	639.37	Joback Method
cpg	559.31	J/molxK	680.72	Joback Method
cpg	579.56	J/molxK	722.06	Joback Method
cpg	599.42	J/molxK	763.41	Joback Method
cpg	619.37	J/molxK	804.76	Joback Method
cpg	639.89	J/molxK	846.10	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R292809&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R292809&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>
<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>

## 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>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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