

# Allyl ionone

**Inchi:** InChI=1S/C15H22O/c1-5-7-13(16)9-10-14-12(2)8-6-11-15(14,3)4/h5,9-10H,1,6-8,11H2,2  
**InchiKey:** ZJPWCCFZZGCMKF-MDZDMXLPSA-N  
**Formula:** C15H22O  
**SMILES:** C=CCC(=O)C=CC1=C(C)CCCC1(C)C  
**Mol. weight [g/mol]:** 218.33

## Physical Properties

Property code	Value	Unit	Source
gf	144.22	kJ/mol	Joback Method
hf	-118.46	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	55.91	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	1679.00		NIST Webbook
rinpol	1605.00		NIST Webbook
ripol	1993.00		NIST Webbook
tb	626.22	K	Joback Method
tc	842.11	K	Joback Method
tf	358.98	K	Joback Method
vc	0.759	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.02	J/molxK	626.22	Joback Method
cpg	536.32	J/molxK	662.20	Joback Method
cpg	553.62	J/molxK	698.18	Joback Method
cpg	570.06	J/molxK	734.16	Joback Method
cpg	585.78	J/molxK	770.14	Joback Method
cpg	600.92	J/molxK	806.12	Joback Method
cpg	615.61	J/molxK	842.11	Joback Method

# Sources

<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=R119947&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R119947&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>ri<sub>npol</sub>:</b>	Non-polar retention indices
<b>ri<sub>pol</sub>:</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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