

# Junenol

<b>Inchi:</b>	InChI=1S/C15H26O/c1-10(2)12-7-9-15(4)8-5-6-11(3)13(15)14(12)16/h10,12-14,16H,3,5-
<b>InchiKey:</b>	MSJJKJCIFIGTJY-UHFFFAOYSA-N
<b>Formula:</b>	C15H26O
<b>SMILES:</b>	C=C1CCCC2(C)CCC(C(C)C)C(O)C12
<b>Mol. weight [g/mol]:</b>	222.37
<b>CAS:</b>	472-07-1

## Physical Properties

Property code	Value	Unit	Source
gf	41.43	kJ/mol	Joback Method
hf	-330.68	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	64.18	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1603.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1627.50		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1588.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1627.50		NIST Webbook
rinpol	1605.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2052.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2028.00		NIST Webbook
ripol	2052.00		NIST Webbook
tb	654.96	K	Joback Method
tc	859.10	K	Joback Method
tf	355.53	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.74	J/mol×K	654.96	Joback Method
cpg	616.91	J/mol×K	688.98	Joback Method
cpg	636.06	J/mol×K	723.01	Joback Method
cpg	654.29	J/mol×K	757.03	Joback Method
cpg	671.72	J/mol×K	791.05	Joback Method
cpg	688.46	J/mol×K	825.08	Joback Method
cpg	704.61	J/mol×K	859.10	Joback Method

## Sources

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C472071&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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