

# Valerenol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10(9-16)8-13-6-4-11(2)14-7-5-12(3)15(13)14/h8,11,13-14,16H,4-
<b>InchiKey:</b>	KIQXKOUFPHTUQS-XJYRDZPNSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(=CC1CCC(C)C2CCC(C)=C12)CO
<b>Mol. weight [g/mol]:</b>	220.35

## Physical Properties

Property code	Value	Unit	Source
gf	98.46	kJ/mol	Joback Method
hf	-256.11	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1661.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1729.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1655.00		NIST Webbook
tb	669.56	K	Joback Method
tc	870.07	K	Joback Method
tf	347.47	K	Joback Method
vc	0.750	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.51	J/molxK	669.56	Joback Method
cpg	592.58	J/molxK	702.98	Joback Method
cpg	609.62	J/molxK	736.40	Joback Method
cpg	625.71	J/molxK	769.82	Joback Method

cpg	640.89	J/mol×K	803.24	Joback Method
cpg	655.23	J/mol×K	836.66	Joback Method
cpg	668.78	J/mol×K	870.07	Joback Method

## Sources

<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=R203908&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R203908&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.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>

## 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>mvol:</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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