

# Valerenol (cis)

<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-RYKHQPThSA-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
rmpol	1698.00		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/mol×K	669.56	Joback Method
cpg	592.58	J/mol×K	702.98	Joback Method
cpg	609.62	J/mol×K	736.40	Joback Method
cpg	625.71	J/mol×K	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=R225057&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R225057&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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