

# «alpha»-Vetivol

<b>Inchi:</b>	InChI=1S/C15H24O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h8,11,14,16H,5-7,9
<b>InchiKey:</b>	OKGZNXMPKYHFRT-UHFFFAOYSA-N
<b>Formula:</b>	C15H24O
<b>SMILES:</b>	CC(C)=C1CCC2=CC(O)CC(C)C2(C)C1
<b>Mol. weight [g/mol]:</b>	220.35
<b>CAS:</b>	57422-86-3

## Physical Properties

Property code	Value	Unit	Source
gf	55.74	kJ/mol	Joback Method
hf	-276.75	kJ/mol	Joback Method
hfus	21.18	kJ/mol	Joback Method
hvap	66.54	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.840		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	1755.60		NIST Webbook
rinpol	1755.60		NIST Webbook
tb	671.57	K	Joback Method
tc	881.76	K	Joback Method
tf	370.77	K	Joback Method
vc	0.744	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.72	J/molxK	671.57	Joback Method
cpg	591.29	J/molxK	706.60	Joback Method
cpg	608.94	J/molxK	741.63	Joback Method
cpg	625.83	J/molxK	776.66	Joback Method
cpg	642.07	J/molxK	811.69	Joback Method
cpg	657.79	J/molxK	846.72	Joback Method
cpg	673.14	J/molxK	881.76	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=C57422863&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57422863&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>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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