

# Veltonal

<b>Inchi:</b>	InChI=1S/C14H22O/c1-11(10-15)7-8-13-12(2)6-5-9-14(13,3)4/h6-8,10-11,13H,5,9H2,1-4
<b>InchiKey:</b>	AISADLWIINCFJS-BQYQJAHWSA-N
<b>Formula:</b>	C14H22O
<b>SMILES:</b>	CC1=CCCC(C)(C)C1C=CC(C)C=O
<b>Mol. weight [g/mol]:</b>	206.32

## Physical Properties

Property code	Value	Unit	Source
gf	76.84	kJ/mol	Joback Method
hf	-210.40	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	52.97	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.760		Crippen Method
mcvol	190.230	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
rinqol	1595.00		NIST Webbook
tb	591.36	K	Joback Method
tc	805.25	K	Joback Method
tf	309.78	K	Joback Method
vc	0.727	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.61	J/molxK	591.36	Joback Method
cpg	508.79	J/molxK	627.01	Joback Method
cpg	526.87	J/molxK	662.66	Joback Method
cpg	543.97	J/molxK	698.31	Joback Method
cpg	560.22	J/molxK	733.95	Joback Method
cpg	575.75	J/molxK	769.60	Joback Method
cpg	590.67	J/molxK	805.25	Joback Method

# Sources

<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>
<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=R589267&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R589267&amp;Units=SI</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>mccvol:</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

Latest version available from:

<https://www.chemeo.com/cid/43-957-2/Veltonal.pdf>

Generated by Cheméo on 2024-04-23 06:39:44.316651777 +0000 UTC m=+16143633.237229092.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.