

# Veloutone

<b>Inchi:</b>	InChI=1S/C13H24O/c1-5-6-7-8-13(4)10-9-12(2,3)11(13)14/h5-10H2,1-4H3
<b>InchiKey:</b>	PUKWIVZFEZFBAT-UHFFFAOYSA-N
<b>Formula:</b>	C13H24O
<b>SMILES:</b>	CCCCC1(C)CCC(C)(C)C1=O
<b>Mol. weight [g/mol]:</b>	196.33

## Physical Properties

Property code	Value	Unit	Source
gf	-46.15	kJ/mol	Joback Method
hf	-378.73	kJ/mol	Joback Method
hfus	11.35	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.962		Crippen Method
mvol	184.740	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rmpol	1306.00		NIST Webbook
rmpol	1306.00		NIST Webbook
tb	575.75	K	Joback Method
tc	788.11	K	Joback Method
tf	358.95	K	Joback Method
vc	0.707	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.15	J/molxK	575.75	Joback Method
cpg	505.06	J/molxK	611.14	Joback Method
cpg	523.94	J/molxK	646.54	Joback Method
cpg	541.98	J/molxK	681.93	Joback Method
cpg	559.33	J/molxK	717.32	Joback Method
cpg	576.17	J/molxK	752.72	Joback Method
cpg	592.67	J/molxK	788.11	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=R607048&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R607048&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>hvp:</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>rinp:</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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