

# Cyclopentanecarboxamide, cis-3-acetoxymethyl-

<b>Inchi:</b>	InChI=1S/C9H15NO3/c1-6(11)13-5-7-2-3-8(4-7)9(10)12/h7-8H,2-5H2,1H3,(H2,10,12)/t7-
<b>InchiKey:</b>	JWBPGWFJMMFYAX-JGVFFNPUSA-N
<b>Formula:</b>	C9H15NO3
<b>SMILES:</b>	CC(=O)OCC1CCC(C(N)=O)C1
<b>Mol. weight [g/mol]:</b>	185.22

## Physical Properties

Property code	Value	Unit	Source
gf	-242.65	kJ/mol	Joback Method
hf	-512.54	kJ/mol	Joback Method
hfus	23.66	kJ/mol	Joback Method
hvap	62.12	kJ/mol	Joback Method
log10ws	-1.07		Crippen Method
logp	0.451		Crippen Method
mcvol	145.800	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	618.62	K	Joback Method
tc	836.51	K	Joback Method
tf	403.20	K	Joback Method
vc	0.538	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.89	J/molxK	618.62	Joback Method
cpg	407.80	J/molxK	654.94	Joback Method
cpg	421.81	J/molxK	691.25	Joback Method
cpg	434.92	J/molxK	727.57	Joback Method
cpg	447.15	J/molxK	763.88	Joback Method
cpg	458.52	J/molxK	800.20	Joback Method
cpg	469.03	J/molxK	836.51	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=B6010450&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010450&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>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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