

# Reposal

**Inchi:** InChI=1S/C14H18N2O3/c1-2-14(11(17)15-13(19)16-12(14)18)10-6-4-8-3-5-9(10)7-8/h6,8  
**InchiKey:** MKELYWOVSPVORM-UHFFFAOYSA-N  
**Formula:** C14H18N2O3  
**SMILES:** CCC1(C2=CCC3CCC2C3)C(=O)NC(=O)NC1=O  
**Mol. weight [g/mol]:** 262.31

## Physical Properties

Property code	Value	Unit	Source
gf	11.24	kJ/mol	Joback Method
hf	-420.62	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Joback Method
hvap	73.42	kJ/mol	Joback Method
log10ws	-2.70		Estimated Solubility Method
logp	1.495		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	866.23	K	Joback Method
tc	1146.26	K	Joback Method
tf	735.66	K	Joback Method
vc	0.730	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	667.03	J/mol×K	866.23	Joback Method
cpg	687.51	J/mol×K	912.90	Joback Method
cpg	706.77	J/mol×K	959.57	Joback Method
cpg	724.90	J/mol×K	1006.25	Joback Method
cpg	742.00	J/mol×K	1052.92	Joback Method
cpg	758.20	J/mol×K	1099.59	Joback Method
cpg	773.60	J/mol×K	1146.26	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>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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Estimated Solubility Method:</b>	<a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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>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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