

# tolcyclamide

<b>Inchi:</b>	InChI=1S/C14H20N2O3S/c1-11-7-9-13(10-8-11)20(18,19)16-14(17)15-12-5-3-2-4-6-12/h
<b>InchiKey:</b>	RIGBPMDIGYBTBJ-UHFFFAOYSA-N
<b>Formula:</b>	C14H20N2O3S
<b>SMILES:</b>	<chem>Cc1ccc(S(=O)(=O)NC(=O)NC2CCCCC2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	296.39

## Physical Properties

Property code	Value	Unit	Source
gf	-224.45	kJ/mol	Joback Method
hf	-511.90	kJ/mol	Joback Method
hfus	40.68	kJ/mol	Joback Method
hvap	88.38	kJ/mol	Joback Method
log10ws	-4.21		Aqueous Solubility Prediction Method
logp	2.316		Crippen Method
mcvol	223.120	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
tb	772.92	K	Joback Method
tc	998.82	K	Joback Method
tf	487.67	K	Joback Method
vc	0.847	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	660.94	J/mol×K	772.92	Joback Method
cpg	677.14	J/mol×K	810.57	Joback Method
cpg	691.88	J/mol×K	848.22	Joback Method
cpg	705.18	J/mol×K	885.87	Joback Method
cpg	717.09	J/mol×K	923.52	Joback Method
cpg	727.64	J/mol×K	961.17	Joback Method
cpg	736.87	J/mol×K	998.82	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>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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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