

# Urea,1- (4'-tert-butyl-2'-chlorophenyl)-

<b>Inchi:</b>	InChI=1S/C11H15ClN2O/c1-11(2,3)7-4-5-9(8(12)6-7)14-10(13)15/h4-6H,1-3H3,(H3,13,1
<b>InchiKey:</b>	UQKVAFJEQWADBT-UHFFFAOYSA-N
<b>Formula:</b>	C11H15ClN2O
<b>SMILES:</b>	CC(C)(C)c1ccc(NC(N)=O)c(Cl)c1
<b>Mol. weight [g/mol]:</b>	226.70

## Physical Properties

Property code	Value	Unit	Source
gf	152.72	kJ/mol	Joback Method
hf	-106.59	kJ/mol	Joback Method
hfus	26.19	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.128		Crippen Method
mvol	175.860	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	698.49	K	Joback Method
tc	934.72	K	Joback Method
tf	483.38	K	Joback Method
vc	0.651	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.20	J/mol×K	698.49	Joback Method
cpg	470.07	J/mol×K	737.86	Joback Method
cpg	481.95	J/mol×K	777.23	Joback Method
cpg	492.91	J/mol×K	816.61	Joback Method
cpg	503.01	J/mol×K	855.98	Joback Method
cpg	512.34	J/mol×K	895.35	Joback Method
cpg	520.95	J/mol×K	934.72	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=B6009300&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6009300&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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