

# Urea, 1-(2-chloroethyl)-3-(m-chloropheneyl)-

<b>Inchi:</b>	InChI=1S/C9H10Cl2N2O/c10-4-5-12-9(14)13-8-3-1-2-7(11)6-8/h1-3,6H,4-5H2,(H2,12,13)
<b>InchiKey:</b>	IRLDFZCVRIBROP-UHFFFAOYSA-N
<b>Formula:</b>	C9H10Cl2N2O
<b>SMILES:</b>	O=C(NCCCl)Nc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	233.09
<b>CAS:</b>	13908-34-4

## Physical Properties

Property code	Value	Unit	Source
gf	153.68	kJ/mol	Joback Method
hf	-41.15	kJ/mol	Joback Method
hfus	32.91	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.700		Crippen Method
mcvol	159.920	ml/mol	McGowan Method
pc	3261.58	kPa	Joback Method
tb	666.05	K	Joback Method
tc	892.32	K	Joback Method
tf	445.22	K	Joback Method
vc	0.606	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.26	J/molxK	666.05	Joback Method
cpg	381.97	J/molxK	703.76	Joback Method
cpg	391.88	J/molxK	741.47	Joback Method
cpg	401.03	J/molxK	779.19	Joback Method
cpg	409.45	J/molxK	816.90	Joback Method
cpg	417.20	J/molxK	854.61	Joback Method
cpg	424.30	J/molxK	892.32	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908344&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908344&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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