

# Urea, 1-(4-amino-3,5-dichlorophenyl)-3-(2-chloroethyl)-

Inchi:	InChI=1S/C9H10Cl3N3O/c10-1-2-14-9(16)15-5-3-6(11)8(13)7(12)4-5/h3-4H,1-2,13H2,(H
InchiKey:	ZRRXILHBUVFOHG-UHFFFAOYSA-N
Formula:	C9H10Cl3N3O
SMILES:	Nc1c(Cl)cc(NC(=O)NCCCl)cc1Cl
Mol. weight [g/mol]:	282.55
CAS:	13908-36-6

## Physical Properties

Property code	Value	Unit	Source
gf	188.94	kJ/mol	Joback Method
hf	-46.04	kJ/mol	Joback Method
hfus	41.52	kJ/mol	Joback Method
hvap	83.30	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	2.936		Crippen Method
mcvol	182.140	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
tb	785.97	K	Joback Method
tc	1021.87	K	Joback Method
tf	583.44	K	Joback Method
vc	0.683	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.99	J/molxK	785.97	Joback Method
cpg	448.82	J/molxK	825.29	Joback Method
cpg	456.91	J/molxK	864.60	Joback Method
cpg	464.29	J/molxK	903.92	Joback Method
cpg	471.00	J/molxK	943.23	Joback Method
cpg	477.08	J/molxK	982.55	Joback Method
cpg	482.56	J/molxK	1021.87	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>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908366&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908366&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>

# 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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