

# Urea, 1,1'-(methylenedi-p-phenylene)bis[3-(2-chloroethy

Inchi:	InChI=1S/C19H22Cl2N4O2/c20-9-11-22-18(26)24-16-5-1-14(2-6-16)13-15-3-7-17(8-4-15
InchiKey:	NPAPTMFFWIVXJJ-UHFFFAOYSA-N
Formula:	C19H22Cl2N4O2
SMILES:	O=C(NCCCCI)Nc1ccc(Cc2ccc(NC(=O)NCCCCI)cc2)cc1
Mol. weight [g/mol]:	409.31
CAS:	13908-71-9

## Physical Properties

Property code	Value	Unit	Source
gf	390.52	kJ/mol	Joback Method
hf	-28.13	kJ/mol	Joback Method
hfus	64.26	kJ/mol	Joback Method
hvap	111.77	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	3.998		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
tb	1080.72	K	Joback Method
tc	1327.20	K	Joback Method
tf	752.11	K	Joback Method
vc	1.133	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	920.29	J/molxK	1080.72	Joback Method
cpg	929.79	J/molxK	1121.80	Joback Method
cpg	938.39	J/molxK	1162.88	Joback Method
cpg	946.20	J/molxK	1203.96	Joback Method
cpg	953.32	J/molxK	1245.04	Joback Method
cpg	959.85	J/molxK	1286.12	Joback Method
cpg	965.92	J/molxK	1327.20	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C13908719&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>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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