

# 1-1'-(1,4-Cyclohexylene)bis[3-(2-chloroethyl)urea], trans-

<b>Inchi:</b>	InChI=1S/C12H22Cl2N4O2/c13-5-7-15-11(19)17-9-1-2-10(4-3-9)18-12(20)16-8-6-14/h9-
<b>InchiKey:</b>	ZJBVHMDPRPAAGM-MGCOHNPYSA-N
<b>Formula:</b>	C12H22Cl2N4O2
<b>SMILES:</b>	O=C(NCCCCI)NC1CCC(NC(=O)NCCCCI)CC1
<b>Mol. weight [g/mol]:</b>	325.24

## Physical Properties

Property code	Value	Unit	Source
gf	142.76	kJ/mol	Joback Method
hf	-299.79	kJ/mol	Joback Method
hfus	51.73	kJ/mol	Joback Method
hvap	90.43	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	1.374		Crippen Method
mcvol	236.620	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
tb	872.12	K	Joback Method
tc	1089.40	K	Joback Method
tf	598.48	K	Joback Method
vc	0.889	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.16	J/molxK	872.12	Joback Method
cpg	744.92	J/molxK	908.33	Joback Method
cpg	756.56	J/molxK	944.55	Joback Method
cpg	767.11	J/molxK	980.76	Joback Method
cpg	776.63	J/molxK	1016.97	Joback Method
cpg	785.14	J/molxK	1053.19	Joback Method
cpg	792.71	J/molxK	1089.40	Joback Method

# Sources

<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=B6007706&amp;Units=SI&amp;Mask=3FFF">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6007706&amp;Units=SI&amp;Mask=3FFF</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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