

N,n'-bis-(2-chlorocyclohexyl)urea

Inchi:	InChI=1S/C13H22Cl2N2O/c14-9-5-1-3-7-11(9)16-13(18)17-12-8-4-2-6-10(12)15/h9-12H,
InchiKey:	HEBOXYNUDXBKBC-UHFFFAOYSA-N
Formula:	C13H22Cl2N2O
SMILES:	O=C(NC1CCCCC1Cl)NC1CCCCC1Cl
Mol. weight [g/mol]:	293.23

Physical Properties

Property code	Value	Unit	Source
gf	118.06	kJ/mol	Joback Method
hf	-280.81	kJ/mol	Joback Method
hfus	35.43	kJ/mol	Joback Method
hvap	73.16	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.386		Crippen Method
mcvol	218.320	ml/mol	McGowan Method
pc	2252.53	kPa	Joback Method
tb	755.67	K	Joback Method
tc	992.67	K	Joback Method
tf	457.64	K	Joback Method
vc	0.801	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	658.54	J/molxK	755.67	Joback Method
cpg	677.88	J/molxK	795.17	Joback Method
cpg	695.57	J/molxK	834.67	Joback Method
cpg	711.65	J/molxK	874.17	Joback Method
cpg	726.19	J/molxK	913.67	Joback Method
cpg	739.23	J/molxK	953.17	Joback Method
cpg	750.82	J/molxK	992.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008426&Units=SI&Mask=3FFF

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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