N-(2-chloroethyl)-n'-(1-phenylcyclohexyl)urea

Inchi: InChI=1S/C15H21ClN2O/c16-11-12-17-14(19)18-15(9-5-2-6-10-15)13-7-3-1-4-8-13/h1,3-
InchiKey: UMHWXFAYDQMFBR-UHFFFAOYSA-N
Formula: C15H21ClN2O
SMILES: O=C(NCCCl)NC1(c2ccccc2)CCCCC1
Mol. weight [g/mol]: 280.79
CAS: 13908-23-1

Physical Properties

Property code	Value	Unit	Source
gf	244.72	kJ/mol	Joback Method
hf	-68.22	kJ/mol	Joback Method
hfus	30.18	kJ/mol	Joback Method
hvap	74.54	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.384		Crippen Method
mcvol	221.360	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
tb	780.71	K	Joback Method
tc	1020.59	K	Joback Method
tf	501.68	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.05	J/mol×K	780.71	Joback Method
cpg	666.58	J/mol×K	820.69	Joback Method
cpg	683.31	J/mol×K	860.67	Joback Method
cpg	699.42	J/mol×K	900.65	Joback Method
cpg	715.13	J/mol×K	940.63	Joback Method
cpg	730.64	J/mol×K	980.61	Joback Method
cpg	746.13	J/mol×K	1020.59	Joback Method

Sources

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=C13908231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume