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

Inchi: InChI=1S/C12H22Cl2N4O2/c13-5-7-15-11(19)17-9-3-1-2-4-10(9)18-12(20)16-8-6-14/h9-
InchiKey: CMCLQPSPSCZGRS-UHFFFAOYSA-N
Formula: C12H22Cl2N4O2
SMILES: O=C(NCCCl)NC1CCCCC1NC(=O)NCCCl
Mol. weight [g/mol]: 325.24
CAS: 13908-62-8

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/mol×K	872.12	Joback Method
cpg	744.92	J/mol×K	908.33	Joback Method
cpg	756.56	J/mol×K	944.55	Joback Method
cpg	767.11	J/mol×K	980.76	Joback Method
cpg	776.63	J/mol×K	1016.97	Joback Method
cpg	785.14	J/mol×K	1053.19	Joback Method
cpg	792.71	J/mol×K	1089.40	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13908628&Units=SI

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