Urea, 1,1'-p-phenylenebis[3-(2-chloroethyl)-3-nitroso-

Inchi: InChI=1S/C12H14Cl2N6O4/c13-5-7-19(17-23)11(21)15-9-1-2-10(4-3-9)16-12(22)20(18-2

InchiKey: PCLGVSQVYVGFSH-UHFFFAOYSA-N

Formula: C12H14Cl2N6O4

SMILES: O=NN(CCCl)C(=O)Nc1ccc(NC(=O)N(CCCl)N=O)cc1

Mol. weight [g/mol]: 377.18

CAS: 13907-59-0

Physical Properties

Property code	Value	Unit	Source
hf	-416.97	kJ/mol	Joback Method
hvap	102.66	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	3.195		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	2460.47	kPa	Joback Method
tb	940.24	K	Joback Method
tc	1159.34	K	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=C13907590&Units=SI

Legend

hf: Enthalpy of formation 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