Urea, 1-(2-chloroethyl)-1-nitroso-3-phenyl-

Inchi: InChI=1S/C9H10ClN3O2/c10-6-7-13(12-15)9(14)11-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,11,14)
InchiKey: NTFJBCLCDARIRQ-UHFFFAOYSA-N
Formula: C9H10ClN3O2
SMILES: O=NN(CCCl)C(=O)Nc1ccccc1
Mol. weight [g/mol]: 227.65
CAS: 13206-67-2

Physical Properties

Property code	Value	Unit	Source
hf	-168.07	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.441		Crippen Method
mcvol	159.230	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
tb	649.31	K	Joback Method
tc	863.52	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13206672&Units=SI
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

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