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

Inchi: InChI=1S/C12H16ClN3O2/c1-8-6-9(2)11(10(3)7-8)14-12(17)16(15-18)5-4-13/h6-7H,4-5H
InchiKey: FBUJDSPUSQUDOE-UHFFFAOYSA-N
Formula: C12H16ClN3O2
SMILES: Cc1cc(C)c(NC(=O)N(CCCl)N=O)c(C)c1
Mol. weight [g/mol]: 269.73
CAS: 33022-06-9

Physical Properties

Property code	Value	Unit	Source
hf	-264.40	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.366		Crippen Method
mcvol	201.500	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
tb	732.89	K	Joback Method
tc	940.65	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33022069&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

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