Urea, 1,1'-(2,3,5,6-tetramethyl-p-phenylene)bis[3-(2-chlo

Inchi: InChI=1S/C16H22Cl2N6O4/c1-9-10(2)14(20-16(26)24(22-28)8-6-18)12(4)11(3)13(9)19-1

InchiKey: HNZDDWZBVSBOPL-UHFFFAOYSA-N

Formula: C16H22Cl2N6O4

SMILES: Cc1c(C)c(NC(=O)N(CCCl)N=O)c(C)c(C)c1NC(=O)N(CCCl)N=O

Mol. weight [g/mol]: 433.29

CAS: 13907-60-3

Physical Properties

Property code	Value	Unit	Source
hf	-545.41	kJ/mol	Joback Method
hvap	114.21	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	4.428		Crippen Method
mcvol	303.180	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
tb	1051.68	K	Joback Method
tc	1287.59	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13907603&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