N''-(4-chloro-phenyl)-N,N,N',N'-tetramethyl-guanidine

Inchi: InChI=1S/C11H16ClN3/c1-14(2)11(15(3)4)13-10-7-5-9(12)6-8-10/h5-8H,1-4H3
InchiKey: NDKSAYCLPKGOPH-UHFFFAOYSA-N
Formula: C11H16ClN3
SMILES: CN(C)C(=Nc1ccc(Cl)cc1)N(C)C
Mol. weight [g/mol]: 225.72

Physical Properties

Property code	Value	Unit	Source
hf	146.44	kJ/mol	Joback Method
hvap	54.88	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.451		Crippen Method
mcvol	179.970	ml/mol	McGowan Method
pc	2269.73	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	621.61	K	Joback Method
tc	843.89	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=R153036&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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