N-(3-methylphenyl)-N'-(3-chlorophenyl)formamidi

Inchi: InChI=1S/C14H13ClN2/c1-11-4-2-6-13(8-11)16-10-17-14-7-3-5-12(15)9-14/h2-10H,1H3,(
InchiKey: AODWFSZKOOZIHK-UHFFFAOYSA-N
Formula: C14H13ClN2
SMILES: Cc1cccc(NC=Nc2cccc(Cl)c2)c1
Mol. weight [g/mol]: 244.72

Physical Properties

Property code	Value	Unit	Source
hf	237.78	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.420		Crippen Method
mcvol	188.500	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	747.32	K	Joback Method
tc	1002.56	K	Joback Method

Sources

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=R161567&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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