N-(3-Methoxyphenyl)-N'-(3-chlorophenyl)formami

Inchi: InChI=1S/C14H13BrN2O/c1-18-14-7-3-6-13(9-14)17-10-16-12-5-2-4-11(15)8-12/h2-10H,
InchiKey: HWHUSLHWHLCIAJ-UHFFFAOYSA-N
Formula: C14H13BrN2O
SMILES: COc1cccc(NC=Nc2cccc(Br)c2)c1
Mol. weight [g/mol]: 305.17

Physical Properties

Property code	Value	Unit	Source
hf	147.63	kJ/mol	Joback Method
hvap	71.23	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.230		Crippen Method
mcvol	199.630	ml/mol	McGowan Method
pc	2576.72	kPa	Joback Method
rinpol	2458.00		NIST Webbook
tb	798.47	K	Joback Method
tc	1056.88	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=R161532&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