N-(3-Chlorophenyl)-N'-(3-bromophenyl)formamidi

Inchi: InChI=1S/C13H10BrClN2/c14-10-3-1-5-12(7-10)16-9-17-13-6-2-4-11(15)8-13/h1-9H,(H,1
InchiKey: GADNKXSYQVUQKQ-UHFFFAOYSA-N
Formula: C13H10BrClN2
SMILES: Clc1cccc(NC=Nc2cccc(Br)c2)c1
Mol. weight [g/mol]: 309.59

Physical Properties

Property code	Value	Unit	Source
hf	284.75	kJ/mol	Joback Method
hvap	70.98	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.874		Crippen Method
mcvol	191.910	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	790.60	K	Joback Method
tc	1061.23	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=R161512&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