N-Phenyl-N'-3-bromophenylformamidine

Inchi: InChI=1S/C13H11BrN2/c14-11-5-4-8-13(9-11)16-10-15-12-6-2-1-3-7-12/h1-10H,(H,15,16
InchiKey: DOLRUYKOAKIUMX-UHFFFAOYSA-N
Formula: C13H11BrN2
SMILES: Brc1cccc(N=CNc2ccccc2)c1
Mol. weight [g/mol]: 275.14

Physical Properties

Property code	Value	Unit	Source
hf	311.96	kJ/mol	Joback Method
hvap	65.93	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.221		Crippen Method
mcvol	179.670	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	2294.00		NIST Webbook
rinpol	2294.00		NIST Webbook
tb	748.19	K	Joback Method
tc	1016.83	K	Joback Method

Sources

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=R161785&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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