N,N-Dimethyl-N'-(3-bromophenyl)-isobutyramidine

Inchi: InChI=1S/C12H17BrN2/c1-9(2)12(15(3)4)14-11-7-5-6-10(13)8-11/h5-9H,1-4H3/b14-12+
InchiKey: PFSAOUGSCKPYGW-WYMLVPIESA-N
Formula: C12H17BrN2
SMILES: CC(C)C(=Nc1cccc(Br)c1)N(C)C
Mol. weight [g/mol]: 269.18

Physical Properties

Property code	Value	Unit	Source
hf	95.06	kJ/mol	Joback Method
hvap	56.73	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.697		Crippen Method
mcvol	189.340	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1834.00		NIST Webbook
tb	660.34	K	Joback Method
tc	894.89	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=R162357&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