N,N-Dimethyl-N'-(4-bromophenyl)-pivalamidine

Inchi: InChI=1S/C13H19BrN2/c1-13(2,3)12(16(4)5)15-11-8-6-10(14)7-9-11/h6-9H,1-5H3/b15-1
InchiKey: ONCXREIRRKAIMA-NTCAYCPXSA-N
Formula: C13H19BrN2
SMILES: CN(C)C(=Nc1ccc(Br)cc1)C(C)(C)C
Mol. weight [g/mol]: 283.21

Physical Properties

Property code	Value	Unit	Source
hf	70.95	kJ/mol	Joback Method
hvap	58.05	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	4.087		Crippen Method
mcvol	203.430	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1843.00		NIST Webbook
tb	680.43	K	Joback Method
tc	919.06	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=R162486&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

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