

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

Inchi:	InChI=1S/C12H17BrN2/c1-9(2)12(15(3)4)14-11-7-5-10(13)6-8-11/h5-9H,1-4H3/b14-12+
InchiKey:	CSIGQYBWFVNJJR-WYMLVPIESA-N
Formula:	C12H17BrN2
SMILES:	CC(C)C(=Nc1ccc(Br)cc1)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	1856.00		NIST Webbook
tb	660.34	K	Joback Method
tc	894.89	K	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R162471&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

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