

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

Inchi: InChI=1S/C15H15BrN2/c1-18(2)15(12-7-4-3-5-8-12)17-14-10-6-9-13(16)11-14/h3-11H,1
InchiKey: JYXSRHOIVYOYWIK-BMRADRMJSA-N
Formula: C15H15BrN2
SMILES: CN(C)C(=Nc1cccc(Br)c1)c1ccccc1
Mol. weight [g/mol]: 303.20

Physical Properties

Property code	Value	Unit	Source
hf	274.95	kJ/mol	Joback Method
hvap	66.07	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.089		Crippen Method
mcvol	207.850	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
rinsol	2126.00		NIST Webbook
tb	756.10	K	Joback Method
tc	1016.54	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=R158571&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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

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