Formamidine, 3,3-dimethyl-1-(3-bromophenyl)

Other names: N'-(3-bromo-phenyl)-N,N-dimethyl-formamidine
Inchi: InChI=1S/C9H11BrN2/c1-12(2)7-11-9-5-3-4-8(10)6-9/h3-7H,1-2H3/b11-7+
InchiKey: AHXJOPPQNFICNX-YRNVUSSQSA-N
Formula: C9H11BrN2
SMILES: CN(C)C=Nc1cccc(Br)c1
Mol. weight [g/mol]: 227.10

Physical Properties

Property code	Value	Unit	Source
hf	172.05	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-2.69		Crippen Method
logp	2.671		Crippen Method
mcvol	147.070	ml/mol	McGowan Method
pc	3072.75	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	592.26	K	Joback Method
tc	832.25	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118404&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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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