Methanimine, 1-(1-pyrrolidinyl), N-(3-bromophenyl)

Inchi: InChI=1S/C11H13BrN2/c12-10-4-3-5-11(8-10)13-9-14-6-1-2-7-14/h3-5,8-9H,1-2,6-7H2
InchiKey: FNXZUCOKXRQFAF-UHFFFAOYSA-N
Formula: C11H13BrN2
SMILES: Brc1cccc(N=CN2CCCC2)c1
Mol. weight [g/mol]: 253.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	3.205		Crippen Method
mcvol	164.390	ml/mol	McGowan Method
rinpol	2048.00		NIST Webbook
rinpol	2048.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118919&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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