Methanimine, 1-(1-pyrrolidinyl), N-(4-bromophenyl)

Inchi: InChI=1S/C11H13BrN2/c12-10-3-5-11(6-4-10)13-9-14-7-1-2-8-14/h3-6,9H,1-2,7-8H2/b13

InchiKey: ZDMVZMGCMZEGBJ-UKTHLTGXSA-N

Formula: C11H13BrN2

SMILES: Brc1ccc(N=CN2CCCC2)cc1

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	2060.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118979&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices