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

Inchi: InChI=1S/C12H15BrN2/c13-11-5-4-6-12(9-11)14-10-15-7-2-1-3-8-15/h4-6,9-10H,1-3,7-8
InchiKey: JQFCLROWAXRVGB-GXDHUFHOSA-N
Formula: C12H15BrN2
SMILES: Brc1cccc(N=CN2CCCCC2)c1
Mol. weight [g/mol]: 267.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.595		Crippen Method
mcvol	178.480	ml/mol	McGowan Method
rinpol	2102.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118726&Units=SI

Legend

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