

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

Inchi: InChI=1S/C12H15BrN2/c13-11-4-6-12(7-5-11)14-10-15-8-2-1-3-9-15/h4-7,10H,1-3,8-9H2
InchiKey: DEOHQMXRRBPMGV-UHFFFAOYSA-N
Formula: C12H15BrN2
SMILES: BrC1ccc(N=CN2CCCCC2)cc1
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	2126.00		NIST Webbook
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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=R118786&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

Latest version available from:

<https://www.chemeo.com/cid/58-244-7/Methanimine-1-1-piperidiny-N-4-bromophenyl.pdf>

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