

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

Inchi: InChI=1S/C13H18N2/c1-12-5-7-13(8-6-12)14-11-15-9-3-2-4-10-15/h5-8,11H,2-4,9-10H2,
InchiKey: MZCHRSCTODSZCJ-SDNWHVSQSA-N
Formula: C13H18N2
SMILES: Cc1ccc(N=CN2CCCCC2)cc1
Mol. weight [g/mol]: 202.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	3.141		Crippen Method
mcvol	175.070	ml/mol	McGowan Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118815&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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