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

Inchi: InChI=1S/C12H16N2/c1-11-4-6-12(7-5-11)13-10-14-8-2-3-9-14/h4-7,10H,2-3,8-9H2,1H3/

InchiKey: QIAKTGLRQDEWLI-JLHYYAGUSA-N

Formula: C12H16N2

SMILES: Cc1ccc(N=CN2CCCC2)cc1

Mol. weight [g/mol]: 188.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	2.751		Crippen Method
mcvol	160.980	ml/mol	McGowan Method
rinpol	1828.00		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=R119016&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