

Methanimine, 1-(1-pyrrolidiny), 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
rinpola	1828.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpola: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/15-442-4/Methanimine-1-1-pyrrolidiny-N-4-methylphenyl.pdf>

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