Methanimine, 1-(1-pyrrolidinyl), N-(3-methylphenyl)

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

InchiKey: IVCJCBNZFJMSCQ-JLHYYAGUSA-N

Formula: C12H16N2

SMILES: Cc1cccc(N=CN2CCCC2)c1

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	1831.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118959&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.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