

Methanimine, 1-(1-pyrrolidiny), N-(4-chlorophenyl)

Inchi: InChI=1S/C11H13ClN2/c12-10-3-5-11(6-4-10)13-9-14-7-1-2-8-14/h3-6,9H,1-2,7-8H2
InchiKey: FPGHAKRIUKQFKF-UHFFFAOYSA-N
Formula: C11H13ClN2
SMILES: Clc1ccc(N=CN2CCCC2)cc1
Mol. weight [g/mol]: 208.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	3.096		Crippen Method
mcvol	159.130	ml/mol	McGowan Method
rinpol	1956.00		NIST Webbook
rinpol	1956.00		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=R118984&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

Latest version available from:

<https://www.chemeo.com/cid/57-921-6/Methanimine-1-1-pyrrolidiny-N-4-chlorophenyl.pdf>

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