Methanimine, 1-(1-piperidinyl), N-(3-chlorophenyl)

Inchi: InChI=1S/C12H15ClN2/c13-11-5-4-6-12(9-11)14-10-15-7-2-1-3-8-15/h4-6,9-10H,1-3,7-8H

InchiKey: CMXRZGJJPWDQOG-GXDHUFHOSA-N

Formula: C12H15ClN2

SMILES: Clc1cccc(N=CN2CCCCC2)c1

Mol. weight [g/mol]: 222.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	3.486		Crippen Method
mcvol	173.220	ml/mol	McGowan Method
rinpol	2006.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R118731&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