Formamidine, 3,3-hexamethyleno-1-(3-chlorophenyl)

Inchi: InChI=1S/C13H17ClN2/c14-12-6-5-7-13(10-12)15-11-16-8-3-1-2-4-9-16/h5-7,10-11H,1-4

InchiKey: XGVWUGAWYVVSMI-RVDMUPIBSA-N

Formula: C13H17ClN2

SMILES: Clc1cccc(N=CN2CCCCCC2)c1

Mol. weight [g/mol]: 236.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.78		Crippen Method
logp	3.876		Crippen Method
mcvol	187.310	ml/mol	McGowan Method
rinpol	2118.00		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=R118568&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