Formamidine, 3,3-hexamethyleno-1-(4-chlorophenyl)

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

InchiKey: GNQQAFXYDKUBGX-UHFFFAOYSA-N

Formula: C13H17ClN2

SMILES: Clc1ccc(N=CN2CCCCCC2)cc1

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	2133.00		NIST Webbook

Sources

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=R118622&Units=SI

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices