

Formamidine, 3,3-hexamethylene-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=CN2CCCCC2)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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/30-337-4/Formamidine-3-3-hexamethylene-1-3-chlorophenyl.pdf>

Generated by Cheméo on 2024-04-17 03:46:21.293553808 +0000 UTC m=+15614830.214131123.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.