

Formamidine, 3,3-hexamethylene-1-(4-methylphenyl)

Inchi:	InChI=1S/C14H20N2/c1-13-6-8-14(9-7-13)15-12-16-10-4-2-3-5-11-16/h6-9,12H,2-5,10-1
InchiKey:	IHZZHYDCVHIXSZ-UHFFFAOYSA-N
Formula:	C14H20N2
SMILES:	Cc1ccc(N=CN2CCCCC2)cc1
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	3.531		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
rinpole	1988.00		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=R118657&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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