

Formamidine, 3,3-hexamethyleno-1-phenyl

Inchi:	InChI=1S/C13H18N2/c1-2-7-11-15(10-6-1)12-14-13-8-4-3-5-9-13/h3-5,8-9,12H,1-2,6-7,1
InchiKey:	MJGSZSLEPRNGMS-WYMLVPIESA-N
Formula:	C13H18N2
SMILES:	C(=Nc1ccccc1)N1CCCCC1
Mol. weight [g/mol]:	202.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Crippen Method
logp	3.222		Crippen Method
mcvol	175.070	ml/mol	McGowan Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R118682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.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

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