

Formamidine, 3,3-hexamethylene-1-(3-methoxyphenyl)

Inchi: InChI=1S/C14H20N2O/c1-17-14-8-6-7-13(11-14)15-12-16-9-4-2-3-5-10-16/h6-8,11-12H,
InchiKey: OYMPLFBCWKJVDK-NTCAYCPXSA-N
Formula: C14H20N2O
SMILES: COc1cccc(N=CN2CCCCC2)c1
Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.21		Crippen Method
logp	3.231		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
rinpol	2144.00		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=R118588&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

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<https://www.chemeo.com/cid/13-024-0/Formamidine-3-3-hexamethylene-1-3-methoxyphenyl.pdf>

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