

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

Inchi: InChI=1S/C15H22N2O/c1-2-18-15-9-7-14(8-10-15)16-13-17-11-5-3-4-6-12-17/h7-10,13H
InchiKey: JRUUOWUKOXJBMZ-DTQAZKPQSA-N
Formula: C15H22N2O
SMILES: CCOc1ccc(N=CN2CCCCCC2)cc1
Mol. weight [g/mol]: 246.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.63		Crippen Method
logp	3.621		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118637&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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