

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

Inchi: InChI=1S/C15H22N2O/c1-2-18-15-9-7-8-14(12-15)16-13-17-10-5-3-4-6-11-17/h7-9,12-14
InchiKey: CGBLEGCHZRAXKR-DTQAZKPQSA-N
Formula: C15H22N2O
SMILES: CCOc1cccc(N=CN2CCCCC2)c1
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
rinpola	2199.00		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=R118573&Units=SI>

Legend

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

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