

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

Inchi: InChI=1S/C13H17BrN2/c14-12-5-7-13(8-6-12)15-11-16-9-3-1-2-4-10-16/h5-8,11H,1-4,9-
InchiKey: JIAVVXZTEINRSA-UHFFFAOYSA-N
Formula: C13H17BrN2
SMILES: Brc1ccc(N=CN2CCCCC2)cc1
Mol. weight [g/mol]: 281.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	3.985		Crippen Method
mcvol	192.570	ml/mol	McGowan Method
rinpol	2239.00		NIST Webbook
rinpol	2239.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118617&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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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