

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

Inchi: InChI=1S/C13H17N3O2/c17-16(18)13-7-5-12(6-8-13)14-11-15-9-3-1-2-4-10-15/h5-8,11H
InchiKey: ZBOLAJUZHRNMQB-SDNWHVSQSA-N
Formula: C13H17N3O2
SMILES: O=[N+](O)c1ccc(N=CN2CCCCC2)cc1
Mol. weight [g/mol]: 247.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	3.131		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	2475.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118662&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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