

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

Inchi: InChI=1S/C14H20N2/c1-2-7-11-16(10-6-1)13-15-12-14-8-4-3-5-9-14/h3-5,8-9,13H,1-2,6-
InchiKey: ABXXCBMBQXQGB-FYWRMAATSA-N
Formula: C14H20N2
SMILES: C(=NCc1ccccc1)N1CCCCC1
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.41		Crippen Method
logp	3.091		Crippen Method
mcvol	189.160	ml/mol	McGowan Method
rinpol	1918.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118697&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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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