Methanimine, 1-(1-piperidinyl), N-(phenylmethyl)

Inchi: InChI=1S/C13H18N2/c1-3-7-13(8-4-1)11-14-12-15-9-5-2-6-10-15/h1,3-4,7-8,12H,2,5-6,9-

InchiKey: QRXXJZFFJLLGCZ-UHFFFAOYSA-N

Formula: C13H18N2

SMILES: C(=NCc1ccccc1)N1CCCCC1

Mol. weight [g/mol]: 202.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	2.701		Crippen Method
mcvol	175.070	ml/mol	McGowan Method
rinpol	1821.00		NIST Webbook
rinpol	1821.00		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=R118895&Units=SI

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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