

Methanimine, 1-(1-piperidiny), N-(4-methoxyphenyl)

Inchi: InChI=1S/C13H18N2O/c1-16-13-7-5-12(6-8-13)14-11-15-9-3-2-4-10-15/h5-8,11H,2-4,9-10H2
InchiKey: ALTBFMZTFUEBPI-SDNWHVVSQSA-N
Formula: C13H18N2O
SMILES: COc1ccc(N=CN2CCCC2)cc1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	2.841		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
rinsol	2052.00		NIST Webbook

Sources

Crippen Method: https://www.cheméo.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=R118800&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.cheméo.com/cid/16-672-8/Methanimine-1-1-piperidiny-N-4-methoxyphenyl.pdf>

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