

Methanimine, 1-(1-pyrrolidiny), N-(3-methoxyphenyl)

Inchi: InChI=1S/C12H16N2O/c1-15-12-6-4-5-11(9-12)13-10-14-7-2-3-8-14/h4-6,9-10H,2-3,7-8H
InchiKey: YLRSDZWACKZGEG-UHFFFAOYSA-N
Formula: C12H16N2O
SMILES: COc1cccc(N=CN2CCCC2)c1
Mol. weight [g/mol]: 204.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	2.451		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
rinpole	1985.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R118944&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
rinpole: Non-polar retention indices

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<https://www.chemeo.com/cid/51-064-4/Methanimine-1-1-pyrrolidiny-N-3-methoxyphenyl.pdf>

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