Methanimine, 1-(1-pyrrolidinyl), N-(4-ethoxyphenyl)

Inchi: InChI=1S/C13H18N2O/c1-2-16-13-7-5-12(6-8-13)14-11-15-9-3-4-10-15/h5-8,11H,2-4,9-1

InchiKey: QOLGELLQSHMFEK-UHFFFAOYSA-N

Formula: C13H18N2O

SMILES: CCOc1ccc(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
rinpol	2042.00		NIST Webbook

Sources

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=R118999&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices