Methanimine, 1-(1-pyrrolidinyl), N-(3-ethoxyphenyl)

Inchi: InChI=1S/C13H18N2O/c1-2-16-13-7-5-6-12(10-13)14-11-15-8-3-4-9-15/h5-7,10-11H,2-4
InchiKey: MZXJRYNAFDFRGZ-UHFFFAOYSA-N
Formula: C13H18N2O
SMILES: CCOc1cccc(N=CN2CCCC2)c1
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	2034.00		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=R118939&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