

Methanimine, 1-(1-pyrrolidiny), 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
rinpola	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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/59-581-2/Methanimine-1-1-pyrrolidiny-N-3-ethoxyphenyl.pdf>

Generated by Cheméo on 2024-04-26 16:32:57.715665304 +0000 UTC m=+16438426.636242621.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.