

Methanimine, 1-(1-pyrrolidinyl), N-phenyl

Inchi:	InChI=1S/C11H14N2/c1-2-6-11(7-3-1)12-10-13-8-4-5-9-13/h1-3,6-7,10H,4-5,8-9H2/b12-
InchiKey:	MWTQWWPBLJONRI-ZRDIBKRKSA-N
Formula:	C11H14N2
SMILES:	C(=Nc1ccccc1)N1CCCC1
Mol. weight [g/mol]:	174.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.26		Crippen Method
logp	2.442		Crippen Method
mcvol	146.890	ml/mol	McGowan Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R119081&Units=SI

Legend

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

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