

Methanimine, 1-(1-pyrrolidiny), N-butyl

Inchi:	InChI=1S/C9H18N2/c1-2-3-6-10-9-11-7-4-5-8-11/h9H,2-8H2,1H3/b10-9+
InchiKey:	YOPOWBBKUXLRLJ-MDZDMXLPSA-N
Formula:	C9H18N2
SMILES:	CCCCN=CN1CCCC1
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.71		Crippen Method
logp	1.911		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
rinpol	1320.00		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=R119036&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

Latest version available from:

<https://www.chemeo.com/cid/35-078-7/Methanimine-1-1-pyrrolidiny-N-butyl.pdf>

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