

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

Inchi:	InChI=1S/C9H18N2/c1-9(2)7-10-8-11-5-3-4-6-11/h8-9H,3-7H2,1-2H3/b10-8+
InchiKey:	SZGVVPYOGFLFKMRC-CSKARUKUSA-N
Formula:	C9H18N2
SMILES:	CC(C)CN=CN1CCCC1
Mol. weight [g/mol]:	154.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.47		Crippen Method
logp	1.766		Crippen Method
mcvol	142.470	ml/mol	McGowan Method
rinpol	1249.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R119061&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/31-971-9/Methanimine-1-1-pyrrolidiny-N-isobutyl.pdf>

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