

2-Pyrrolidinethione, 1-methyl-

Other names:	N-Methyl-2-thiopyrrolidinone
Inchi:	InChI=1S/C5H9NS/c1-6-4-2-3-5(6)7/h2-4H2,1H3
InchiKey:	OQILOJRSIWGQSM-UHFFFAOYSA-N
Formula:	C5H9NS
SMILES:	CN1CCCC1=S
Mol. weight [g/mol]:	115.20
CAS:	10441-57-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.23		Crippen Method
logp	1.039		Crippen Method
mcvol	92.480	ml/mol	McGowan Method

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=C10441573&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/88-043-7/2-Pyrrolidinethione-1-methyl.pdf>

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