

1-Methyl-3-pyrrolidinol

Other names:	N-Methyl-3-pyrrolidinol 3-Pyrrolidinol, 1-methyl- 1-methylpyrrolidin-3-ol
Inchi:	InChI=1S/C5H11NO/c1-6-3-2-5(7)4-6/h5,7H,2-4H2,1H3
InchiKey:	FLVFPAIGVBQGET-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CN1CCC(O)C1
Mol. weight [g/mol]:	101.15
CAS:	13220-33-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.24		Crippen Method
logp	-0.317		Crippen Method
mcvol	86.300	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	324.20	K	0.10	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=C13220332&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
tbrp:	Boiling point at reduced pressure

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