

1,2-Dimethyl-pyrrolidine

Other names:	Pyrrolidine, 1,2-dimethyl- N,2-dimethylpyrrolidine
Inchi:	InChI=1S/C6H13N/c1-6-4-3-5-7(6)2/h6H,3-5H2,1-2H3
InchiKey:	PXHHIBMOFPCBJQ-UHFFFAOYSA-N
Formula:	C6H13N
SMILES:	CC1CCCN1C
Mol. weight [g/mol]:	99.17
CAS:	765-48-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.91		Crippen Method
logp	1.101		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
rinpol	722.00		NIST Webbook
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rinpol	722.00		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=C765480&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

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<https://www.chemeo.com/cid/73-029-9/1-2-Dimethyl-pyrrolidine.pdf>

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