

1,2,2-Trimethyl-pyrrolidine

Inchi:	InChI=1S/C7H15N/c1-7(2)5-4-6-8(7)3/h4-6H2,1-3H3
InchiKey:	STDJRYDBFFDKCR-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CN1CCCC1(C)C
Mol. weight [g/mol]:	113.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.33		Crippen Method
logp	1.491		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
rinpol	798.00		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=R405560&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
rinpol:	Non-polar retention indices

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<https://www.chemeo.com/cid/30-100-6/1-2-2-Trimethyl-pyrrolidine.pdf>

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