

1H-Pyrrole, 1,2-dimethyl

Other names:	1,2-Dimethylpyrrole
Inchi:	InChI=1S/C6H9N/c1-6-4-3-5-7(6)2/h3-5H,1-2H3
InchiKey:	GNFLFHZJXXFDRA-UHFFFAOYSA-N
Formula:	C6H9N
SMILES:	Cc1cccn1C
Mol. weight [g/mol]:	95.14
CAS:	600-29-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	1.334		Crippen Method
mcvol	85.920	ml/mol	McGowan Method
rinpol	876.00		NIST Webbook
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1229.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C600293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

ripol: Polar retention indices

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