

1H-Pyrrole, 1-propyl-

Other names:	Pyrrole, 1-propyl 1-propylpyrrole
Inchi:	InChI=1S/C7H11N/c1-2-5-8-6-3-4-7-8/h3-4,6-7H,2,5H2,1H3
InchiKey:	MFGOZCIHXVFZBC-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	CCCN1CCCC1
Mol. weight [g/mol]:	109.17
CAS:	5145-64-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.15		Crippen Method
logp	1.898		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
rinpol	879.00		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	889.00		NIST Webbook
ripol	1258.00		NIST Webbook
ripol	1251.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C5145642&Units=SI

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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