

Pyrrolidine, 1-propyl-

Other names:	N-propyl-Tetrahydropyrrole 1-Propyl-pyrrolidine
Inchi:	InChI=1S/C7H15N/c1-2-5-8-6-3-4-7-8/h2-7H2,1H3
InchiKey:	HLNRRPIYRBBHSQ-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	CCCN1CCCC1
Mol. weight [g/mol]:	113.20
CAS:	7335-07-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.22		Crippen Method
logp	1.492		Crippen Method
mcpol	108.610	ml/mol	McGowan Method
ripol	882.00		NIST Webbook
ripol	857.00		NIST Webbook
ripol	847.00		NIST Webbook
ripol	839.00		NIST Webbook
ripol	882.00		NIST Webbook
ripol	848.00		NIST Webbook
ripol	838.00		NIST Webbook
ripol	1007.00		NIST Webbook
ripol	987.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7335071&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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