1-[1(1H)-pyrrolyl]-2-propanone

Inchi:	InChI=1S/C7H9NO/c1-7(9)6-8-4-2-3-5-8/h2-5H,6H2,1H3
InchiKey:	YVBZZCOVACFNOO-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	CC(=O)Cn1cccc1
Mol. weight [g/mol]:	123.15

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.43		Crippen Method
logp	1.077		Crippen Method
mcvol	101.580	ml/mol	McGowan Method
rinpol	1037.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R227622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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