

# 1-(1'-pyrrolidinyI)-2-propanone

**Other names:** 1-(1-pyrrolidinyI)-2-propanone  
**Inchi:** InChI=1S/C7H13NO/c1-7(9)6-8-4-2-3-5-8/h2-6H2,1H3  
**InchiKey:** YZZYFRBPGIXHPD-UHFFFAOYSA-N  
**Formula:** C7H13NO  
**SMILES:** CC(=O)CN1CCCC1  
**Mol. weight [g/mol]:** 127.18

## Physical Properties

Property code	Value	Unit	Source
log10ws	-0.50		Crippen Method
logp	0.671		Crippen Method
mcvol	110.180	ml/mol	McGowan Method
ripol	1410.00		NIST Webbook
ripol	1410.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U366036&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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  
**ripol:** Polar retention indices

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