1-(1'-pyrrolidinyl)-2-propanone

Other names: 1-(1-pyrrolidinyl)-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/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
ripol: Polar retention indices