

2-Acetyl-3-(1-pyrrolidinyl)furan

Inchi:	InChI=1S/C10H13NO2/c1-8(12)10-9(4-7-13-10)11-5-2-3-6-11/h4,7H,2-3,5-6H2,1H3
InchiKey:	ZMZXULGNHHLJMN-UHFFFAOYSA-N
Formula:	C10H13NO2
SMILES:	CC(=O)c1occc1N1CCCC1
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.51		Crippen Method
logp	2.082		Crippen Method
mcvol	138.860	ml/mol	McGowan Method
ripol	2347.00		NIST Webbook
ripol	2347.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R532464&Units=SI
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

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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<https://www.chemeo.com/cid/94-376-1/2-Acetyl-3-1-pyrrolidinyl-furan.pdf>

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