

1-(1'-pyrrolidinyI)-2-butanone

Other names:	1-(1-pyrrolidinyI)-2-butanone
Inchi:	InChI=1S/C8H15NO/c1-2-8(10)7-9-5-3-4-6-9/h2-7H2,1H3
InchiKey:	FKJHJSJBXISMIR-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	CCC(=O)CN1CCCC1
Mol. weight [g/mol]:	141.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.92		Crippen Method
logp	1.061		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
ripol	1481.00		NIST Webbook
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Sources

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=U366038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/91-864-2/1-1-pyrrolidinyI-2-butanone.pdf>

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