

Pyrrolidine, 1-(1-oxopropyl)-

Other names:	Pyrrolidine, 1-propionyl- N-Propionylpyrrolidine Pyrrolidine, N-propanoyl
Inchi:	InChI=1S/C7H13NO/c1-2-7(9)8-5-3-4-6-8/h2-6H2,1H3
InchiKey:	YEJJUJNTWYKFLS-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	CCC(=O)N1CCCC1
Mol. weight [g/mol]:	127.18
CAS:	4553-05-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.99		Crippen Method
logp	1.019		Crippen Method
mcvol	110.180	ml/mol	McGowan Method

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=C4553053&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/36-040-7/Pyrrolidine-1-1-oxopropyl.pdf>

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