1-(Hydroxymethyl)-2-pyrrolidinone

Other names:	1-(hydroxymethyl)pyrrolidin-2-one
Inchi:	InChI=1S/C5H9NO2/c7-4-6-3-1-2-5(6)8/h7H,1-4H2
InchiKey:	PJEXUIKBGBSHBS-UHFFFAOYSA-N
Formula:	C5H9NO2
SMILES:	O=C1CCCN1CO
Mol. weight [g/mol]:	115.13
CAS:	15438-71-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.09		Crippen Method
logp	-0.441		Crippen Method
mcvol	87.870	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=C15438718&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/98-385-7/1-Hydroxymethyl-2-pyrrolidinone.pdf

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