

Hygrine

Other names:	2-Propanone, 1-(1-methyl-2-pyrrolidiny)-, (R)- N-Methyl-2-acetonylpyrrolidine, (R)-
Inchi:	InChI=1S/C8H15NO/c1-7(10)6-8-4-3-5-9(8)2/h8H,3-6H2,1-2H3/t8-/m1/s1
InchiKey:	ADKXZIOQKHHDNQ-MRVPVSSYSA-N
Formula:	C8H15NO
SMILES:	CC(=O)CC1CCCN1C
Mol. weight [g/mol]:	141.21
CAS:	496-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	1.060		Crippen Method
mcvol	124.270	ml/mol	McGowan Method
rinpol	1060.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1320.10		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1060.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=C496491&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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