1-Propanone, 1-(2-pyridinyl)-

Other names:	1-Propanone, 1-(2-pyridyl)-
	2-Propionylpyridine
	2-Pyridyl ethyl ketone
	1-(2-pyridinyl)-1-propanone
Inchi:	InChI=1S/C8H9NO/c1-2-8(10)7-5-3-4-6-9-7/h3-6H,2H2,1H3
InchiKey:	ZHAZHKPVEROFLH-UHFFFAOYSA-N
Formula:	C8H9NO
SMILES:	CCC(=O)c1ccccn1
Mol. weight [g/mol]:	135.16
CAS:	3238-55-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	1.674		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
rinpol	1102.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1165.00		NIST Webbook
ripol	1676.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3238559&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices