1-Pentanone, 1-(2-pyridinyl)-

Other names: 1-Pentanone, 1-(2-pyridyl)-
Inchi: InChI=1S/C10H13NO/c1-2-3-7-10(12)9-6-4-5-8-11-9/h4-6,8H,2-3,7H2,1H3
InchiKey: DGBHHRPKPZCABG-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCCCC(=O)c1ccccn1
Mol. weight [g/mol]: 163.22
CAS: 7137-97-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.15		Crippen Method
logp	2.454		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
rinpol	1297.00		NIST Webbook
rinpol	1297.00		NIST Webbook

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=C7137975&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
rinpol: Non-polar retention indices

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