5-(4-Oxopentanoyl)-6-methyl-2,3-dihydro-1H-pyrro

Inchi: InChI=1S/C13H17NO2/c1-9(15)5-6-13(16)12-8-11-4-3-7-14(11)10(12)2/h8H,3-7H2,1-2H
InchiKey: CYIKLYFTXYTIFO-UHFFFAOYSA-N
Formula: C13H17NO2
SMILES: CC(=O)CCC(=O)c1cc2n(c1C)CCC2
Mol. weight [g/mol]: 219.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	2.295		Crippen Method
mcvol	176.830	ml/mol	McGowan Method
ripol	2820.00		NIST Webbook
ripol	2820.00		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=R312037&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
ripol: Polar retention indices

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