1-(5-methyl-2-furanyl)-4-pentanone

Inchi: InChI=1S/C10H14O2/c1-8(11)4-3-5-10-7-6-9(2)12-10/h6-7H,3-5H2,1-2H3
InchiKey: BYXWQTYYVMPQMN-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(=O)CCCc1ccc(C)o1
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	2.500		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
ripol	1769.00		NIST Webbook
ripol	1769.00		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=R296678&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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