1-(2-furanyl)-3-pentanone

Inchi: InChI=1S/C9H12O2/c1-2-8(10)5-6-9-4-3-7-11-9/h3-4,7H,2,5-6H2,1H3
InchiKey: AMBBSXGLKUJWPV-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CCC(=O)CCc1ccco1
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.54		Crippen Method
logp	2.191		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
ripol	1701.00		NIST Webbook
ripol	1701.00		NIST Webbook
ripol	1701.00		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=R296643&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