1-Pentanone, 1-(2-furanyl)-

Other names: Furan, 2-pentanoyl
Inchi: InChI=1S/C9H12O2/c1-2-3-5-8(10)9-6-4-7-11-9/h4,6-7H,2-3,5H2,1H3
InchiKey: HTOZHTBIOGGHDJ-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CCCCC(=O)c1ccco1
Mol. weight [g/mol]: 152.19
CAS: 3194-17-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	2.652		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1180.00		NIST Webbook
rinpol	1180.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1747.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3194170&Units=SI

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