1-(5-methyl-2-furyl)-2-propanone

Inchi: InChI=1S/C8H10O2/c1-6(9)5-8-4-3-7(2)10-8/h3-4H,5H2,1-2H3
InchiKey: BDIRNQMRQINOKT-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: CC(=O)Cc1ccc(C)o1
Mol. weight [g/mol]: 138.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.18		Crippen Method
logp	1.720		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1047.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1566.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1564.00		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=R230792&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