1-(dimethyl-2-furyl)-2-propanone

Inchi: InChI=1S/C9H12O2/c1-6-4-8(3)11-9(6)5-7(2)10/h4H,5H2,1-3H3
InchiKey: NHRKAWBWWHOVHU-UHFFFAOYSA-N
Formula: C9H12O2
SMILES: CC(=O)Cc1oc(C)cc1C
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.66		Crippen Method
logp	2.028		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1151.00		NIST Webbook
rinpol	1151.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R238607&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.