3-Acetyl-2,5-dimethyl furan

Other names: Ethanone, 1-(2,5-dimethyl-3-furanyl)-
Furan, 3-acetyl-2,5-dimethyl
1-(2,5-dimethyl-3-furyl)ethan-1-one
Inchi: InChI=1S/C8H10O2/c1-5-4-8(6(2)9)7(3)10-5/h4H,1-3H3
InchiKey: KBSVBCHYXYXDAG-UHFFFAOYSA-N
Formula: C8H10O2
SMILES: CC(=O)c1cc(C)oc1C
Mol. weight [g/mol]: 138.16
CAS: 10599-70-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.82		Crippen Method
logp	2.099		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
rinpol	1103.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1118.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10599709&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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