4-Acetyl-3,4(5)-dimethylpyridine

Inchi: InChI=1S/C9H11NO/c1-6-4-10-5-7(2)9(6)8(3)11/h4-5H,1-3H3
InchiKey: ZKJBKKNRSCBIPT-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: CC(=O)c1c(C)cncc1C
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	1.901		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
ripol	1892.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1893.00		NIST Webbook
ripol	1894.00		NIST Webbook
ripol	1892.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533105&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
ripol: Polar retention indices