2-Acetyl-4,6-dimethylpyridine

Inchi: InChI=1S/C9H11NO/c1-6-4-7(2)10-9(5-6)8(3)11/h4-5H,1-3H3
InchiKey: IWZFETYQIYPLIE-UHFFFAOYSA-N
Formula: C9H11NO
SMILES: CC(=O)c1cc(C)cc(C)n1
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	1720.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1720.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R533056&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

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