

4-Acetyl-2-methylpyridine

Inchi: InChI=1S/C8H9NO/c1-6-5-8(7(2)10)3-4-9-6/h3-5H,1-2H3
InchiKey: NIGBUKPEJHINOG-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: CC(=O)c1ccnc(C)c1
Mol. weight [g/mol]: 135.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.593		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
ripol	1816.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1818.00		NIST Webbook
ripol	1816.00		NIST Webbook

Sources

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=R533096&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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