5-Acetyl-2-methylpyridine

Other names: 1-(6-Methyl-3-pyridyl)-1-ethanone
Pyridine, 5-acetyl-2-methyl
Inchi: InChI=1S/C8H9NO/c1-6-3-4-8(5-9-6)7(2)10/h3-5H,1-2H3
InchiKey: PVRYOKQFLBSILA-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: CC(=O)c1ccc(C)nc1
Mol. weight [g/mol]: 135.16
CAS: 42972-46-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	1.593		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
rinpol	1189.00		NIST Webbook
rinpol	1162.00		NIST Webbook
rinpol	1189.00		NIST Webbook
ripol	1876.00		NIST Webbook
ripol	1902.00		NIST Webbook
ripol	1876.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42972463&Units=SI

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