Acetic acid, (1-methyl-2(1H)-pyridinylidene)-, methyl ester

Inchi: InChI=1S/C9H11NO2/c1-10-6-4-3-5-8(10)7-9(11)12-2/h3-7H,1-2H3/b8-7+
InchiKey: BRIRBMVQJSWOKR-BQYQJAHWSA-N
Formula: C9H11NO2
SMILES: COC(=O)C=C1C=CC=CN1C
Mol. weight [g/mol]: 165.19
CAS: 39998-21-5

Physical Properties

Property code	Value	Unit	Source
ie	7.02 ± 0.02	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.059		Crippen Method
mcvol	131.330	ml/mol	McGowan Method

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=C39998215&Units=SI

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.