3-Pyridineacetic acid, 1,4-dihydro-1-methyl-, methyl ester

Inchi: InChI=1S/C9H13NO2/c1-10-5-3-4-8(7-10)6-9(11)12-2/h3,5,7H,4,6H2,1-2H3
InchiKey: YMGFECXAXAXEOP-UHFFFAOYSA-N
Formula: C9H13NO2
SMILES: COC(=O)CC1=CN(C)C=CC1
Mol. weight [g/mol]: 167.21
CAS: 39998-23-7

Physical Properties

Property code	Value	Unit	Source
ie	6.94 ± 0.02	eV	NIST Webbook
log10ws	-1.61		Crippen Method
logp	1.283		Crippen Method
mcvol	135.630	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=C39998237&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.