Methyl 1-methyl-1,2-dihydropyridine-3-carboxylate

Inchi: InChI=1S/C8H11NO2/c1-9-5-3-4-7(6-9)8(10)11-2/h3-5H,6H2,1-2H3
InchiKey: CGYIFFSHZMZBES-UHFFFAOYSA-N
Formula: C8H11NO2
SMILES: COC(=O)C1=CC=CN(C)C1
Mol. weight [g/mol]: 153.18
CAS: 19355-19-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.70		Crippen Method
logp	0.545		Crippen Method
mcvol	121.540	ml/mol	McGowan Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		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=C19355192&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