Picolinic acid N-oxide, methyl ester

Inchi: InChI=1S/C7H7NO3/c1-11-7(9)6-4-2-3-5-8(6)10/h2-5H,1H3
InchiKey: XGHWESXDIVXZKH-UHFFFAOYSA-N
Formula: C7H7NO3
SMILES: COC(=O)c1cccc[n+]1[O-]
Mol. weight [g/mol]: 153.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	0.107		Crippen Method
mcvol	109.020	ml/mol	McGowan Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U352499&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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