2-Pyridyl-1,2-ethanediol

Inchi: InChI=1S/C7H9NO2/c9-5-7(10)6-3-1-2-4-8-6/h1-4,7,9-10H,5H2
InchiKey: ORRCHBGKENHRKA-UHFFFAOYSA-N
Formula: C7H9NO2
SMILES: OCC(O)c1ccccn1
Mol. weight [g/mol]: 139.15
CAS: 3944-00-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.03		Crippen Method
logp	0.107		Crippen Method
mcvol	107.450	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3944001&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