Pyridine, 4-phenoxy-, 1-oxide

Inchi: InChI=1S/C11H9NO2/c13-12-8-6-11(7-9-12)14-10-4-2-1-3-5-10/h1-9H
InchiKey: TYEPZEMCJSMYDJ-UHFFFAOYSA-N
Formula: C11H9NO2
SMILES: [O-][n+]1ccc(Oc2ccccc2)cc1
Mol. weight [g/mol]: 187.19
CAS: 33399-53-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	2.112		Crippen Method
mcvol	140.050	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=C33399530&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