4-Pyridinepropionic acid

Inchi: InChI=1S/C8H9NO2/c10-8(11)2-1-7-3-5-9-6-4-7/h3-6H,1-2H2,(H,10,11)
InchiKey: WSXGQYDHJZKQQB-UHFFFAOYSA-N
Formula: C8H9NO2
SMILES: O=C(O)CCc1ccncc1
Mol. weight [g/mol]: 151.16
CAS: 6318-43-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.56		Crippen Method
logp	1.099		Crippen Method
mcvol	117.240	ml/mol	McGowan Method

Sources

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=C6318430&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume