3-Pyridinepropionic acid

Other names:	Pyridine-3-propionic acid
Inchi:	InChI=1S/C8H9NO2/c10-8(11)4-3-7-2-1-5-9-6-7/h1-2,5-6H,3-4H2,(H,10,11)
InchiKey:	WDGXIUUWINKTGP-UHFFFAOYSA-N
Formula:	C8H9NO2
SMILES:	O=C(O)CCc1cccnc1
Mol. weight [g/mol]:	151.16
CAS:	3724-19-4

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:	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=C3724194&Units=SI

Legend

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