

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

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/ci9903071
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

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<https://www.chemeo.com/cid/60-219-2/4-Pyridinepropionic-acid.pdf>

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