

Alpha-hydroxy-4-pyridinemethanesulfonic acid

Inchi:	InChI=1S/C6H7NO4S/c8-6(12(9,10)11)5-1-3-7-4-2-5/h1-4,6,8H,(H,9,10,11)
InchiKey:	LQGYKYJLWSWUAR-UHFFFAOYSA-N
Formula:	C6H7NO4S
SMILES:	O=S(=O)([O-])C(O)c1cc[nH+]cc1
Mol. weight [g/mol]:	189.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.20		Crippen Method
logp	-1.445		Crippen Method
mcvol	121.450	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=B6008579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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