

# 4-Pyridineethanesulfonic acid

<b>Other names:</b>	2-(4-Pyridyl)ethanesulfonic acid 4-Pyridyl-2-ethyl sulfonic acid «beta»-(4-Pyridyl)ethanesulfonic acid 4-Pyridylethylsulfonic acid 2-(4-pyridyl)ethanesulphonic acid
<b>Inchi:</b>	InChI=1S/C7H9NO3S/c9-12(10,11)6-3-7-1-4-8-5-2-7/h1-2,4-5H,3,6H2,(H,9,10,11)
<b>InchiKey:</b>	RGIIAYDCZSXHGL-UHFFFAOYSA-N
<b>Formula:</b>	C7H9NO3S
<b>SMILES:</b>	O=S(=O)(O)CCc1ccncc1
<b>Mol. weight [g/mol]:</b>	187.22
<b>CAS:</b>	53054-76-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	0.512		Crippen Method
mcvol	129.670	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C53054765&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C53054765&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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