

Pyridine, 2-(methylsulfonyl)-

Inchi:	InChI=1S/C6H7NO2S/c1-10(8,9)6-4-2-3-5-7-6/h2-5H,1H3
InchiKey:	PCLKVJBRTCQNDU-UHFFFAOYSA-N
Formula:	C6H7NO2S
SMILES:	CS(=O)(=O)c1ccccn1
Mol. weight [g/mol]:	157.19
CAS:	17075-14-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.93		Crippen Method
logp	0.485		Crippen Method
mcvol	109.710	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=C17075148&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/52-981-5/Pyridine-2-methylsulfonyl.pdf>

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