

Thiazole, 5-acetamido-2-(methylsulfonyl)-

Inchi:	InChI=1S/C6H8N2O3S2/c1-4(9)8-5-3-7-6(12-5)13(2,10)11/h3H,1-2H3,(H,8,9)
InchiKey:	VIIYGBWERIGQKQ-UHFFFAOYSA-N
Formula:	C6H8N2O3S2
SMILES:	CC(=O)Nc1cnc(S(C)=O)=O)s1
Mol. weight [g/mol]:	220.27
CAS:	116529-24-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.89		Crippen Method
logp	0.505		Crippen Method
mcvol	141.910	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116529249&Units=SI

Legend

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

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