

# Thiazole, 5-acetamido-2-(methylsulfonyl)-4-nitro-

Inchi:	InChI=1S/C6H7N3O5S2/c1-3(10)7-5-4(9(11)12)8-6(15-5)16(2,13)14/h1-2H3,(H,7,10)
InchiKey:	JXRPQZUGBAJILT-UHFFFAOYSA-N
Formula:	C6H7N3O5S2
SMILES:	CC(=O)Nc1sc(S(C)=O)=O)nc1[N+](=O)[O-]
Mol. weight [g/mol]:	265.27
CAS:	116529-25-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.413		Crippen Method
mcvol	159.330	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116529250&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116529250&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

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