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: 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=C116529250&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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