1-Methyl-4-nitro-5-(o-acetamidophenylsulfinyl)imi

Inchi: InChI=1S/C12H12N4O4S/c1-8(17)14-9-5-3-4-6-10(9)21(20)12-11(16(18)19)13-7-15(12)2
InchiKey: UACSPGWZIHFVIT-UHFFFAOYSA-N
Formula: C12H12N4O4S
SMILES: CC(=O)Nc1ccccc1S(=O)c1c([N+](=O)[O-])ncn1C
Mol. weight [g/mol]: 308.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	1.453		Crippen Method
mcvol	207.870	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=B6008345&Units=SI

Legend

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