# Imidazol-5-yl,1-methyl-4-nitro-p-acetamidophenyl

**Inchi:** InChI=1S/C12H12N4O5S/c1-8(17)14-9-3-5-10(6-4-9)22(20,21)12-11(16(18)19)13-7-15(1
**InchiKey:** WMBLBOVKDMARBZ-UHFFFAOYSA-N
**Formula:** C12H12N4O5S
**SMILES:** CC(O)=Nc1ccc(S(=O)(=O)c2c([N+](=O)[O-])ncn2C)cc1
**Mol. weight [g/mol]:** 324.31
**CAS:** 5702-78-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.93 | | Crippen Method |
| logp | 1.769 | | Crippen Method |
| mcvol | 213.740 | ml/mol | McGowan Method |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C5702783&Units=SI
**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

## Legend

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