

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

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