2-Amino-4-(p-acetamidophenyl)-thiazole

Inchi: InChI=1S/C11H11N3OS/c1-7(15)13-9-4-2-8(3-5-9)10-6-16-11(12)14-10/h2-6H,1H3,(H2,1
InchiKey: VBBNSESFUHRMJU-UHFFFAOYSA-N
Formula: C11H11N3OS
SMILES: CC(=O)Nc1ccc(-c2csc(N)n2)cc1
Mol. weight [g/mol]: 233.29
CAS: 21674-96-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	2.351		Crippen Method
mcvol	170.490	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21674964&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