N-acetyl-n-(p-aminobenzene-sulfonyl)-2-amino-4,6

Inchi: InChI=1S/C14H16N4O3S/c1-9-8-10(2)17-14(16-9)18(11(3)19)22(20,21)13-6-4-12(15)5-7
InchiKey: VRYCOLRKKCBJJI-UHFFFAOYSA-N
Formula: C14H16N4O3S
SMILES: CC(=O)N(c1nc(C)cc(C)n1)S(=O)(=O)c1ccc(N)cc1
Mol. weight [g/mol]: 320.37
CAS: 35255-37-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	1.417		Crippen Method
mcvol	230.180	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35255379&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