

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

<b>Inchi:</b>	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
<b>InchiKey:</b>	VRYCOLRKKCBJJI-UHFFFAOYSA-N
<b>Formula:</b>	C14H16N4O3S
<b>SMILES:</b>	CC(=O)N(c1nc(C)cc(C)n1)S(=O)(=O)c1ccc(N)cc1
<b>Mol. weight [g/mol]:</b>	320.37
<b>CAS:</b>	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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35255379&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35255379&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-785-0/N-acetyl-n-p-aminobenzene-sulfonyl-2-amino-4-6-dimethylpyrimidine.pdf>

Generated by Cheméo on 2024-04-23 11:57:27.370507809 +0000 UTC m=+16162696.291085124.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.