

# [1,2,5]-Thiadiazolo[3,4-d]pyrimidine, 5,7-dipyrrolidin-1-yl-

**Inchi:** InChI=1S/C12H16N6S/c1-2-6-17(5-1)11-9-10(16-19-15-9)13-12(14-11)18-7-3-4-8-18/h1-12  
**InchiKey:** HATWPRLPAYDUNK-UHFFFAOYSA-N  
**Formula:** C12H16N6S  
**SMILES:** C1CCN(c2nc(N3CCCC3)c3nsnc3n2)C1  
**Mol. weight [g/mol]:** 276.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.38		Crippen Method
logp	1.682		Crippen Method
mcvol	195.530	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008331&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

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

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