[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-

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

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/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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