

[1,2,5]Thiadiazolo[3,4-d]pyrimidine, 7-(hydroxyamino)-

Inchi: InChI=1S/C4H3N5OS/c10-7-3-2-4(6-1-5-3)9-11-8-2/h1,10H,(H,5,6,7,9)
InchiKey: NBVJKBQINASAJM-UHFFFAOYSA-N
Formula: C4H3N5OS
SMILES: ONc1ncnc2nsnc12
Mol. weight [g/mol]: 169.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.34		Crippen Method
logp	0.282		Crippen Method
mcvol	100.420	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=B6007718&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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