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

Inchi: InChI=1S/C8H12N6O2S/c15-3-1-9-6-5-7(14-17-13-5)12-8(11-6)10-2-4-16/h15-16H,1-4H

InchiKey: HNYKFFHQQGNDSF-UHFFFAOYSA-N

Formula: C8H12N6O2S

SMILES: OCCNc1nc(NCCO)c2nsnc2n1

Mol. weight [g/mol]: 256.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	-0.710		Crippen Method
mcvol	172.630	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=B6010469&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