

[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:	HNYKFFHQGGNSF-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/ci9903071

Legend

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

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