[1,2,5]Thiadiazolo[3,4-d]pyrimidine, 5-amino-7-butylamino-

Inchi: InChI=1S/C8H12N6S/c1-2-3-4-10-6-5-7(14-15-13-5)12-8(9)11-6/h2-4H2,1H3,(H3,9,10,11

InchiKey: GXCZMRDVTHOASY-UHFFFAOYSA-N

Formula: C8H12N6S

SMILES: CCCCNc1nc(N)nc2nsnc12

Mol. weight [g/mol]: 224.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Crippen Method
logp	1.276		Crippen Method
mcvol	160.890	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=B6008427&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