Benzenesulfonamide, p-[2-(purin-6-ylamino)ethyl]-

Inchi: InChI=1S/C13H14N6O2S/c14-22(20,21)10-3-1-9(2-4-10)5-6-15-12-11-13(17-7-16-11)19-

InchiKey: HNTKMTOFOQSLQA-UHFFFAOYSA-N

Formula: C13H14N6O2S

SMILES: NS(=O)(=O)c1ccc(CCNc2ncnc3nc[nH]c23)cc1

Mol. weight [g/mol]: 318.35

CAS: 21266-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	0.173		Crippen Method
mcvol	219.320	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=C21266671&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