

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:	HNTKMTFOQSLQA-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
mvol	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/ci9903071

Legend

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

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<https://www.chemeo.com/cid/115-702-4/Benzenesulfonamide-p-2-purin-6-ylamino-ethyl.pdf>

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