.alpha.-[6-AMINO-9H-PURIN-9-YL]-p-TOLUENESU

Other names: «alpha»-[6-Amino-9H-purin-9-yl]-p-toluenesulfonamide
Inchi: InChI=1S/C12H12N6O2S/c13-11-10-12(16-6-15-11)18(7-17-10)5-8-1-3-9(4-2-8)21(14,19
InchiKey: HYYXGPTXYDTDSM-UHFFFAOYSA-N
Formula: C12H12N6O2S
SMILES: Nc1ncnc2c1ncn2Cc1ccc(S(N)(=O)=O)cc1
Mol. weight [g/mol]: 304.33

Physical Properties

Property code	Value	Unit	Source
logp	0.104		Crippen Method
mcvol	205.230	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21267981&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume