.alpha.-[PURINE-6-YLAMINO]-p-TOLUENESULFO

Other names: «alpha»-[Purine-6-ylamino]-p-toluenesulfonamide
Inchi: InChI=1S/C12H12N6O2S/c13-21(19,20)9-3-1-8(2-4-9)5-14-11-10-12(16-6-15-10)18-7-17
InchiKey: MGZJAXYRCXYPPD-UHFFFAOYSA-N
Formula: C12H12N6O2S
SMILES: NS(=O)(=O)c1ccc(CNc2ncnc3[nH]cnc23)cc1
Mol. weight [g/mol]: 304.33

Physical Properties

Property code	Value	Unit	Source
ie	8.23	eV	Cheméo Relay (1.0)
log10ws	-3.81		Cheméo Relay (1.0)
logp	0.130		Crippen Method
mcvol	205.230	ml/mol	McGowan Method
tf	568.35	K	Cheméo Relay (1.0)

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21266660&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point