

.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:	HYXXGPTXYDTSMD-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

Latest version available from:

<https://www.chemeo.com/cid/29-456-4/alpha-6-AMINO-9H-PURIN-9-YL-p-TOLUENESULFONAMIDE.pdf>

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