

Hypoxanthine, 7-(2-hydroxyethyl)-, p-toluenesulfonate

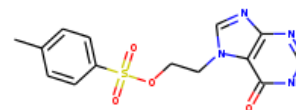
InChI: InChI=1S/C14H14N4O4S/c1-10-2-4-11(5-3-10)23(20,21)22-7-6-18-9-17-13-12(18)14(19)16-8-15-13/h2-5,8-9H,6-7H2,1H3,(H,15,16,19)

InChI Key: XLVQASBAPODVNN-UHFFFAOYSA-N

Formula: C₁₄H₁₄N₄O₄S

SMILES: Cc1ccc(S(=O)(=O)OCCn2cnc3nc[nH]c(=O)c32)cc1

Molecular Weight: 334.35



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	0.834		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H14N4O4S/c1-10-2-4-11\(5-3-10\)23\(20,21\)22-7-6-18-9-17-13-12\(18\)14\(19\)16-8-15-13/h2-5,8-9H,6-7H2,1H3,\(H,15,16,19\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C14H14N4O4S/c1-10-2-4-11(5-3-10)23(20,21)22-7-6-18-9-17-13-12(18)14(19)16-8-15-13/h2-5,8-9H,6-7H2,1H3,(H,15,16,19))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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