

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)
InchiKey: XLVQASBAPODVNN-UHFFFAOYSA-N
Formula: C14H14N4O4S
SMILES: Cc1ccc(S(=O)(=O)OCCn2cnc3nc[nH]c(=O)c32)cc1
Mol. weight [g/mol]: 334.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.19		Crippen Method
logp	0.352		Crippen Method
mcvol	225.190	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=B6009925&Units=SI>

Legend

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

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