Hypoxanthine, 1-benzyl-9-cyclopentyl-

Inchi: InChI=1S/C17H18N4O/c22-17-15-16(21(12-18-15)14-8-4-5-9-14)19-11-20(17)10-13-6-2-
InchiKey: JPRIVYHVLKRNDI-UHFFFAOYSA-N
Formula: C17H18N4O
SMILES: O=c1c2ncn(C3CCCC3)c2ncn1Cc1ccccc1
Mol. weight [g/mol]: 294.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.16		Crippen Method
logp	2.756		Crippen Method
mcvol	222.640	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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=B6008204&Units=SI

Legend

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