

Hypoxanthine-7-ethanol, 2,3-dihydro-3-(diphenylmethyl)-, acetate

Inchi: InChI=1S/C22H24N4O3/c1-16(27)29-13-12-25-14-23-21-20(25)22(28)24-15-26(21)19(17)
InchiKey: IBPKENMWIWUBAJ-UHFFFAOYSA-N
Formula: C22H24N4O3
SMILES: CC(=O)OCCn1cnc2c1C(O)NCN2C(c1cccc1)c1cccc1
Mol. weight [g/mol]: 392.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	2.594		Crippen Method
mcvol	296.230	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=B6009933&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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