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(c1ccccc1)c1ccccc1

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/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=B6009933&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume