Hypoxanthine-7-ethanol, alpha-acetate

Inchi: InChI=1S/C9H10N4O3/c1-6(14)16-3-2-13-5-12-8-7(13)9(15)11-4-10-8/h4-5H,2-3H2,1H3,
InchiKey: NVBBFXNWTAENQF-UHFFFAOYSA-N
Formula: C9H10N4O3
SMILES: CC(=O)OCCn1cnc2nc[nH]c(=O)c21
Mol. weight [g/mol]: 222.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	-0.799		Crippen Method
mcvol	151.980	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=B6008015&Units=SI

Legend

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