Thiazolo[3,2-a]pyridinium, 8-(acetyloxy)-3-hydroxy-2-phenyl-, hydroxide, inner salt

Other names: Thiazolo[3,2-a]pyridinium, 3,8-dihydroxy-2-phenyl-, hydroxide, inner salt, 8-acetate
Inchi: InChI=1S/C15H11NO3S/c1-10(17)19-12-8-5-9-16-14(18)13(20-15(12)16)11-6-3-2-4-7-11
InchiKey: VPLIRLQTSUXSIV-UHFFFAOYSA-N
Formula: C15H11NO3S
SMILES: CC(=O)Oc1ccc[n+]2c([O-])c(-c3ccccc3)sc12
Mol. weight [g/mol]: 285.32
CAS: 32002-92-9

Physical Properties

Property code	Value	Unit	Source
ie	6.27 ± 0.05	eV	NIST Webbook
log10ws	-8.20		Crippen Method
logp	2.153		Crippen Method
mcvol	199.170	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=C32002929&Units=SI

Legend

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