

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)11-6-3-2-4-7-1
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/ci9903071
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

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