Thiazolo[3,2-a]pyridinium, 3-hydroxy-2-phenyl-, hydroxide, inner salt

Inchi: InChI=1S/C13H9NOS/c15-13-12(10-6-2-1-3-7-10)16-11-8-4-5-9-14(11)13/h1-9H
InchiKey: QATLDNWNHCIBKT-UHFFFAOYSA-N
Formula: C13H9NOS
SMILES: [O-]c1c(-c2ccccc2)sc2cccc[n+]12
Mol. weight [g/mol]: 227.28
CAS: 32044-03-4

Physical Properties

Property code	Value	Unit	Source
ie	6.70 ± 0.05	eV	NIST Webbook
log10ws	-7.89		Crippen Method
logp	2.227		Crippen Method
mcvol	163.550	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32044034&Units=SI
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

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.