Thiazolo[3,2-a]pyridinium, 2,3-dihydro-8-hydroxy-, hydroxide, inner salt

Other names: Dihydrothiazolo[3,2-a]pyridinium 8-oxide
Inchi: InChI=1S/C7H7NOS/c9-6-2-1-3-8-4-5-10-7(6)8/h1-3H,4-5H2
InchiKey: UQOJAMOQNDLMOU-UHFFFAOYSA-N
Formula: C7H7NOS
SMILES: [O-]c1ccc[n+]2c1SCC2
Mol. weight [g/mol]: 153.20
CAS: 23003-45-4

Physical Properties

Property code	Value	Unit	Source
ie	7.12 ± 0.05	eV	NIST Webbook
log10ws	-5.05		Crippen Method
logp	0.153		Crippen Method
mcvol	107.070	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23003454&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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