Thiazolo[3,2-a]pyridinium, 2,3-dihydro-8-hydroxy-5-methyl-, hydroxide, inner salt

Inchi: InChI=1S/C8H9NOS/c1-6-2-3-7(10)8-9(6)4-5-11-8/h2-3H,4-5H2,1H3
InchiKey: IJQXSEDDFABXPP-UHFFFAOYSA-N
Formula: C8H9NOS
SMILES: Cc1ccc([O-])c2[n+]1CCS2
Mol. weight [g/mol]: 167.23
CAS: 23003-43-2

Physical Properties

Property code	Value	Unit	Source
ie	6.93 ± 0.05	eV	NIST Webbook
ie	6.95 ± 0.05	eV	NIST Webbook
ie	7.35 ± 0.05	eV	NIST Webbook
log10ws	-5.52		Crippen Method
logp	0.462		Crippen Method
mcvol	121.160	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=C23003432&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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