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

Inchi: InChI=1S/C8H7NOS/c1-6-5-11-8-7(10)3-2-4-9(6)8/h2-5H,1H3
InchiKey: KJOMNERCZAHBEJ-UHFFFAOYSA-N
Formula: C8H7NOS
SMILES: Cc1csc2c([O-])ccc[n+]12
Mol. weight [g/mol]: 165.21
CAS: 30276-99-4

Physical Properties

Property code	Value	Unit	Source
ie	7.12 ± 0.05	eV	NIST Webbook
log10ws	-5.76		Crippen Method
logp	0.869		Crippen Method
mcvol	116.860	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=C30276994&Units=SI

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.