Thiazolo[3,2-a]pyridinium,3,8-dihydroxy-,hydroxid
salt

Inchi: InChI=1S/C7H5NO2S/c9-5-2-1-3-8-6(10)4-11-7(5)8/h1-4,10H
InchiKey: WJDNUMGWKKKHHV-UHFFFAOYSA-N
Formula: C7H5NO2S
SMILES: [O-]c1ccc[n+]2c(O)csc12
Mol. weight [g/mol]: 167.19
CAS: 35143-55-6

Physical Properties

Property code	Value	Unit	Source
ie	8.70 ± 0.05	eV	NIST Webbook
log10ws	-4.83		Crippen Method
logp	0.266		Crippen Method
mcvol	108.640	ml/mol	McGowan Method

Sources

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=C35143556&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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