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

Inchi: InChI=1S/C9H9NOS/c1-6-3-4-8(11)9-10(6)7(2)5-12-9/h3-5H,1-2H3
InchiKey: VSJUEYWEHFPCSS-UHFFFAOYSA-N
Formula: C9H9NOS
SMILES: Cc1ccc([O-])c2scc(C)[n+]12
Mol. weight [g/mol]: 179.24
CAS: 30277-00-0

Physical Properties

Property code	Value	Unit	Source
ie	6.84 ± 0.05	eV	NIST Webbook
log10ws	-6.24		Crippen Method
logp	1.177		Crippen Method
mcvol	130.950	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=C30277000&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

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