

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

Inchi: InChI=1S/C8H7NOS/c1-6-2-3-7(10)8-9(6)4-5-11-8/h2-5H,1H3
InchiKey: DESPLGBYAU LRQC-UHFFFAOYSA-N
Formula: C8H7NOS
SMILES: Cc1ccc([O-])c2scc[n+]12
Mol. weight [g/mol]: 165.21
CAS: 30277-17-9

Physical Properties

Property code	Value	Unit	Source
ie	7.03 ± 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/ci9903071>
Crippen Method: https://www.cheméo.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=C30277179&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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