Thiazolo[3,2-c]pyrimidin-4-ium, 2,3-dihydro-8-hydroxy-5-methyl-, hydroxide, inner salt

Inchi: InChI=1S/C7H8N2OS/c1-5-8-4-6(10)7-9(5)2-3-11-7/h4H,2-3H2,1H3
InchiKey: LXPWRJJEUZZNLC-UHFFFAOYSA-N
Formula: C7H8N2OS
SMILES: Cc1ncc([O-])c2[n+]1CCS2
Mol. weight [g/mol]: 168.22
CAS: 24614-07-1

Physical Properties

Property code	Value	Unit	Source
ie	7.40 ± 0.05	eV	NIST Webbook
log10ws	-5.29		Crippen Method
logp	-0.143		Crippen Method
mcvol	117.050	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24614071&Units=SI
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

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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