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

**Inchi:** InChI=1S/C8H9NOS/c1-6-2-3-7(10)8-9(6)4-5-11-8/h2-3H,4-5H2,1H3
**InchiKey:** IJQXSEDDFABXPP-UHFFFAOYSA-N
**Formula:** C8H9NOS
**SMILES:** Cc1ccc([O-])c2[n+]1CCS2
**Mol. weight [g/mol]:** 167.23
**CAS:** 23003-43-2

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 6.93 ± 0.05 | eV | NIST Webbook |
| ie | 6.95 ± 0.05 | eV | NIST Webbook |
| ie | 7.35 ± 0.05 | eV | NIST Webbook |
| log10ws | -5.52 | | Crippen Method |
| logp | 0.462 | | Crippen Method |
| mcvol | 121.160 | 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=C23003432&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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