Thiazolo[3,2-a]pyridinium, 3,8-dihydroxy-2-phenyl-, hydroxide, inner salt

Inchi: InChI=1S/C13H9NO2S/c15-10-7-4-8-14-12(16)11(17-13(10)14)9-5-2-1-3-6-9/h1-8H,(H-,1

InchiKey: LATUNNOOSZTYQB-UHFFFAOYSA-N

Formula: C13H9NO2S

SMILES: [O-]c1c(-c2ccccc2)sc2c(O)ccc[n+]12

Mol. weight [g/mol]: 243.28

CAS: 35143-57-8

Physical Properties

Property code	Value	Unit	Source
ie	8.42 ± 0.05	eV	NIST Webbook
log10ws	-7.44		Crippen Method
logp	1.933		Crippen Method
mcvol	169.420	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=C35143578&Units=SI

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.