Acridine 10-oxide

Other names: Acridine-N-oxide
Inchi: InChI=1S/C13H9NO/c15-14-12-7-3-1-5-10(12)9-11-6-2-4-8-13(11)14/h1-9H
InchiKey: HYGIWTYYBBTQAL-UHFFFAOYSA-N
Formula: C13H9NO
SMILES: [O-][n+]1c2ccccc2cc2ccccc21
Mol. weight [g/mol]: 195.22
CAS: 10399-73-2

Physical Properties

Property code	Value	Unit	Source
ie	7.45 ± 0.02	eV	NIST Webbook
log10ws	-6.61		Crippen Method
logp	2.626		Crippen Method
mcvol	147.200	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10399732&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