

Acridophosphine, 10-methyl-

Inchi: InChI=1S/C14H11P/c1-10-11-6-2-4-8-13(11)15-14-9-5-3-7-12(10)14/h2-9H,1H3
InchiKey: BXPBJWHVMRQMSG-UHFFFAOYSA-N
Formula: C14H11P
SMILES: Cc1c2ccccc2pc2ccccc12
Mol. weight [g/mol]: 210.21
CAS: 57422-79-4

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| ie | 7.19 | eV | NIST Webbook |
| log10ws | -2.55 | | Crippen Method |
| logp | 4.882 | | Crippen Method |
| mcvol | 165.900 | ml/mol | McGowan Method |

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C57422794&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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