

# Phosphoramidous acid, phenyl-, diethyl ester

|                             |                                                                               |
|-----------------------------|-------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C10H16NO2P/c1-3-12-14(13-4-2)11-10-8-6-5-7-9-10/h5-9,11H,3-4H2,1-2H3 |
| <b>InchiKey:</b>            | AOSDIQRAKHSDQA-UHFFFAOYSA-N                                                   |
| <b>Formula:</b>             | C10H16NO2P                                                                    |
| <b>SMILES:</b>              | CCOP(Nc1ccccc1)OCC                                                            |
| <b>Mol. weight [g/mol]:</b> | 213.21                                                                        |
| <b>CAS:</b>                 | 5156-98-9                                                                     |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | 0.26    |        | Crippen Method |
| logp          | 3.398   |        | Crippen Method |
| mcvol         | 170.180 | ml/mol | McGowan Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5156989&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5156989&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |

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