

2-[4-(diethoxyphosphorylmethyl)phenyl]-1,3-benz

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|-----------------------------|---|
| Inchi: | InChI=1S/C18H20NO3PS/c1-3-21-23(20,22-4-2)13-14-9-11-15(12-10-14)18-19-16-7-5-6 |
| InchiKey: | FVYRUSCZCWSFLT-UHFFFAOYSA-N |
| Formula: | C18H20NO3PS |
| SMILES: | CCOP(=O)(Cc1ccc(-c2nc3ccccc3s2)cc1)OCC |
| Mol. weight [g/mol]: | 361.40 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| log10ws | -4.00 | | Aqueous Solubility Prediction Method |
| logp | 5.729 | | Crippen Method |
| mcvol | 266.200 | ml/mol | McGowan Method |

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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